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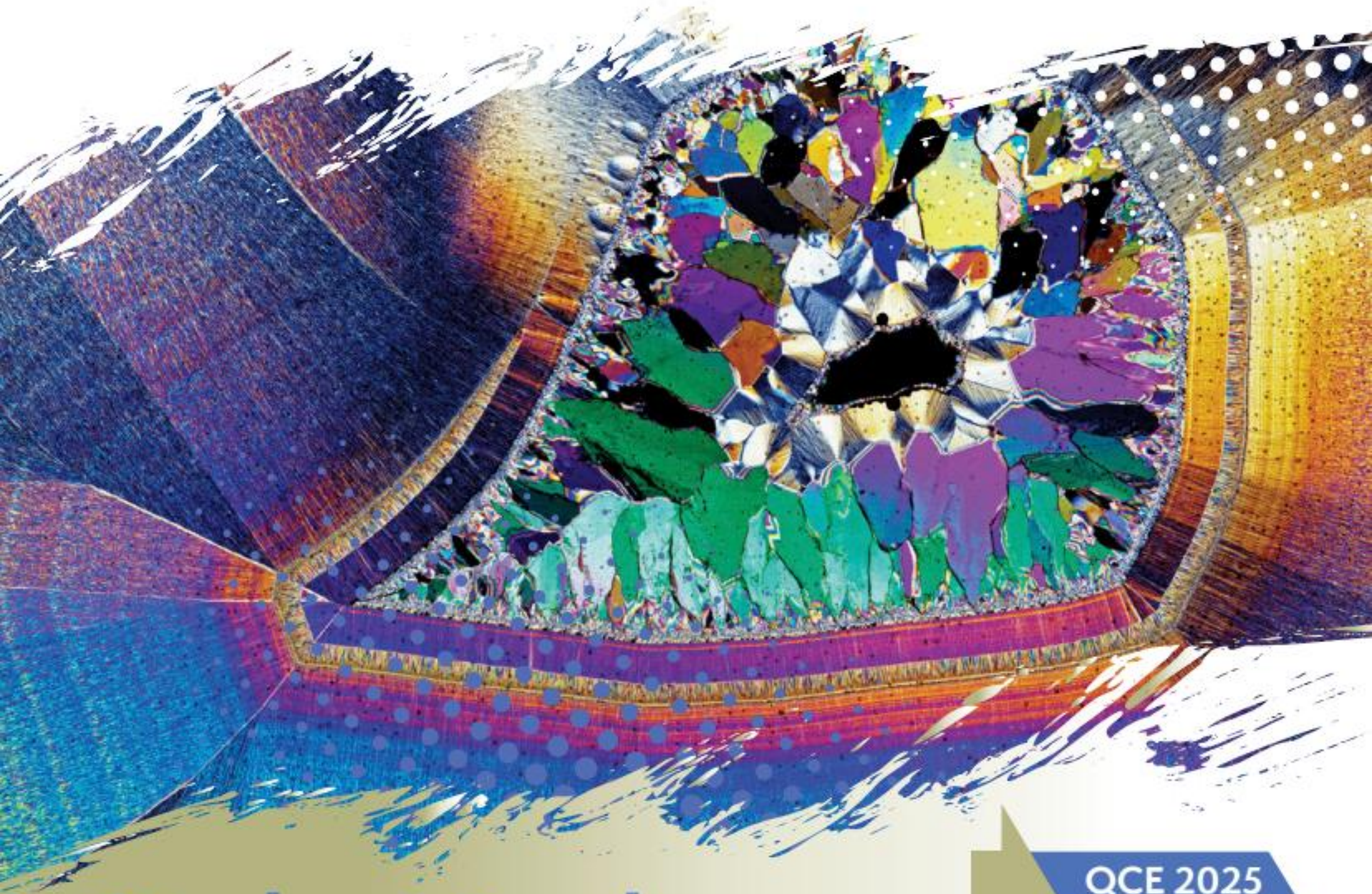
UNITS 1 & 2



Student Book

QCE 2025 Chemistry SYLLABUS

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STUDENT BOOK

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Chemistry General Senior Syllabus 2025 © State of Queensland (QCAA) 2024.

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The Chemistry Education Association (CEA) was formed in 1977 by a group of teachers from secondary and tertiary institutions. It aims to promote the teaching of chemistry, particularly in secondary schools.

The CEA has established a tradition of providing up-to-date text, electronic material and support resources for both students and teachers, and professional development opportunities for teachers.

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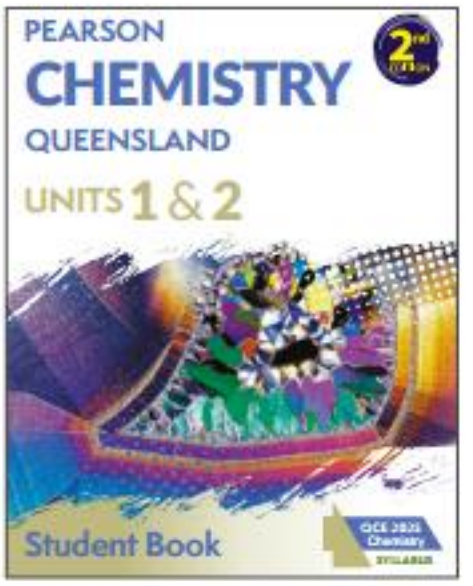

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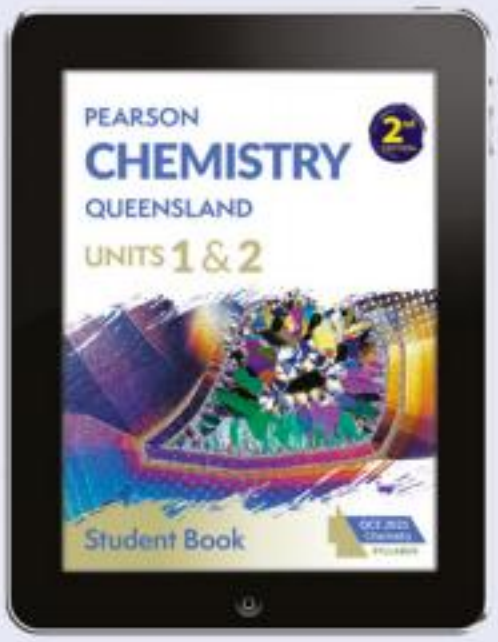

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How to use this book

PEARSON CHEMISTRY QUEENSLAND STUDENT BOOK UNITS 1 & 2 2ND EDITION

Pearson Chemistry Queensland Student Book Units 1 & 2nd edition has been written to the 2025 QCAA Chemistry Syllabus. This book includes an additional Skills and Assessment Toolkit online as well as a depth of additional resources, to support every aspect of teaching and learning. Explore how to use this book below.

Design

Featuring best-practice literacy and instructional design, this series supports all learners with careful scaffolding of concepts and defined learning objectives.

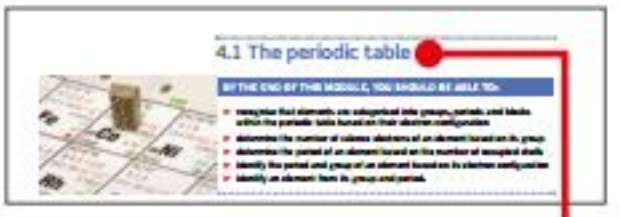
A simple to navigate, predictable design enables ease of use. The high-quality, relevant photos and illustrations assist student understanding of concepts.

Chapter 1

The Skills and Assessment Toolkit provides support across the Science Inquiry Skills and Assessment requirements. The material is presented as a handy reference to enable confident, complete coverage of the syllabus across the course. Reworked and fully updated to meet the evolved requirements of the revised QCE 2025 Syllabus, and to respond to the needs of teachers and students.

Chapter opener

The syllabus subject matter addressed in each chapter is clearly listed, and mapped to the modules in which the content is addressed.



Module opener

Module openers outline the key concepts and skills developed and link to syllabus subject matter listed in the Chapter opener.

Highlight box

Highlight features focus on important information such as key definitions, formulas and salient points.

Skillbuilder

A Skillbuilder outlines a method or technique. Each is instructive and self-contained. Skillbuilders step students through the skills to support science application, supporting development of key science inquiry skills.

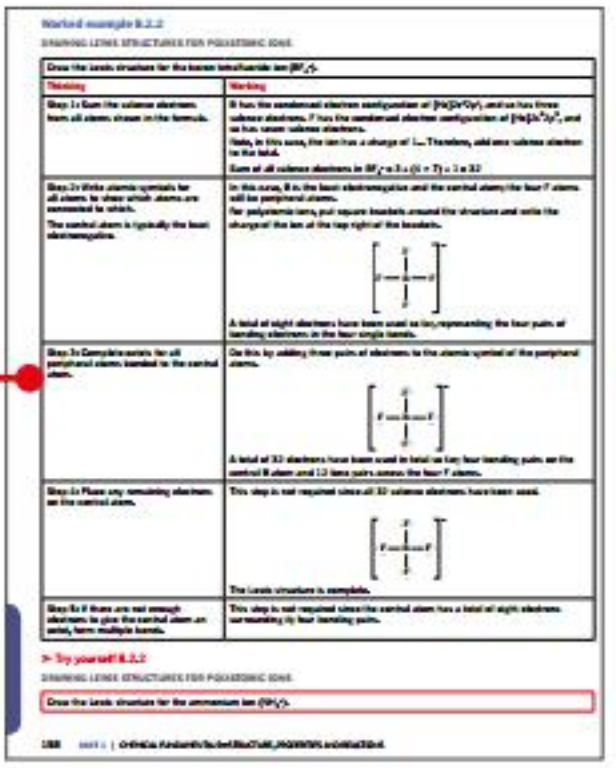
Science as a Human Endeavour

Science as a Human Endeavour features provide stimulus for the Research Investigation. The SHE features are structured to develop the foundational skills relevant to supporting the relevant science inquiry skills through the lens of science as a human endeavour, providing a suitable foundation from which students can launch into Research Investigation IA3 and draw upon building proficiency for the Assessment objectives 1, 2 and 3.

Worked Examples

Worked Examples use sequential steps of thinking and working to model a best-practice approach to scaffolding student development of subject matter. This research-based approach greatly enhances student understanding and application of formulas to subject matter. Each Worked Example is followed by a Try Yourself task where students apply their learning to a mirrored problem to practise the skill.

Fully worked solutions to all Try Yourself problems are available from *Pearson Chemistry Queensland Units 1 & 2 2nd edition eBook*.

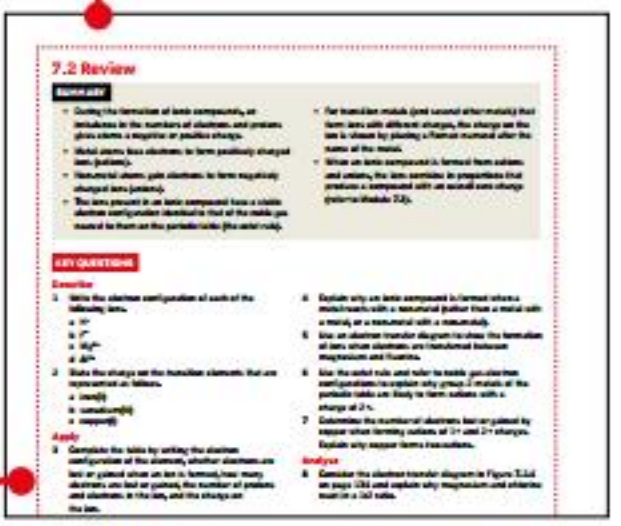


Module review

Key instructions are provided to test students' understanding of concepts of the module. Questions are presented under the four Assessment Objectives of Describe, Apply and Analyse. This structure allows students to demonstrate their progress in developing an understanding of the science subject matter.

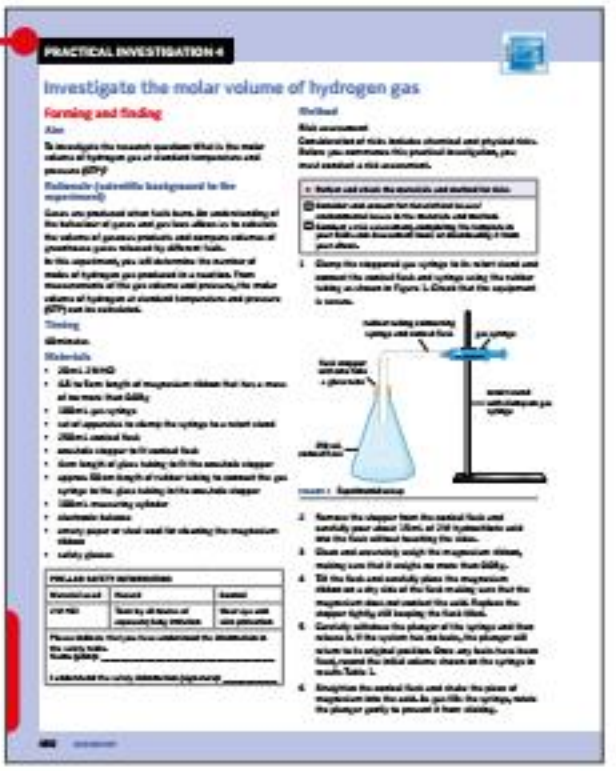
Module summary

Each module concludes with a summary to help students consolidate the key points and concepts.



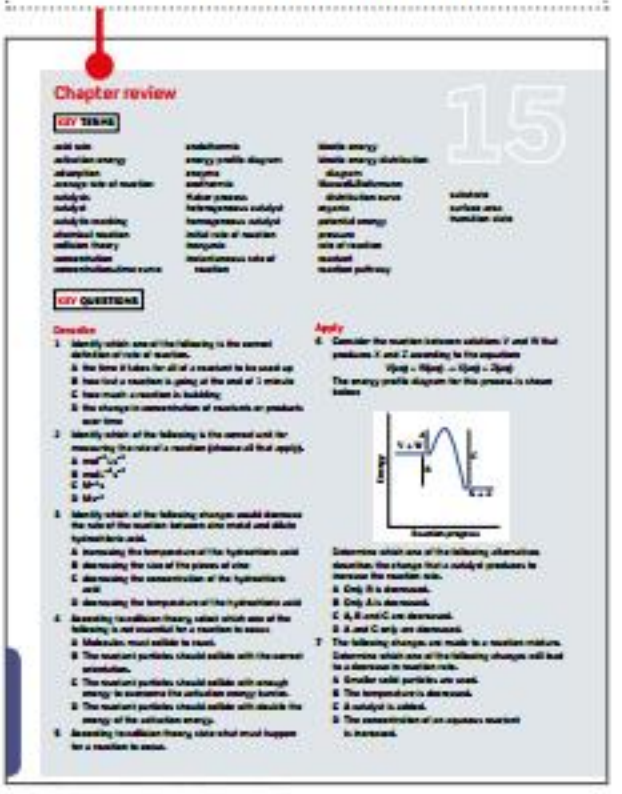
Practical Manual

Practical Investigations offer students the opportunity to develop, practise and refine their science inquiry skills. These activities involve gathering primary data to analyse and respond to scaffolded or open-ended science tasks, supporting deeper understanding and proficiency in scientific methods. Additionally, these tasks allow teachers to formatively assess students' science inquiry skills and set students up well with the insights for Student experiment IA2, pertinent to Assessment objectives 1 to 6. All Practical Investigations have been trialled and tested to ensure they can be safely performed and yield effective results. Full risk assessments and additional support are provided in the eBook.



Chapter review

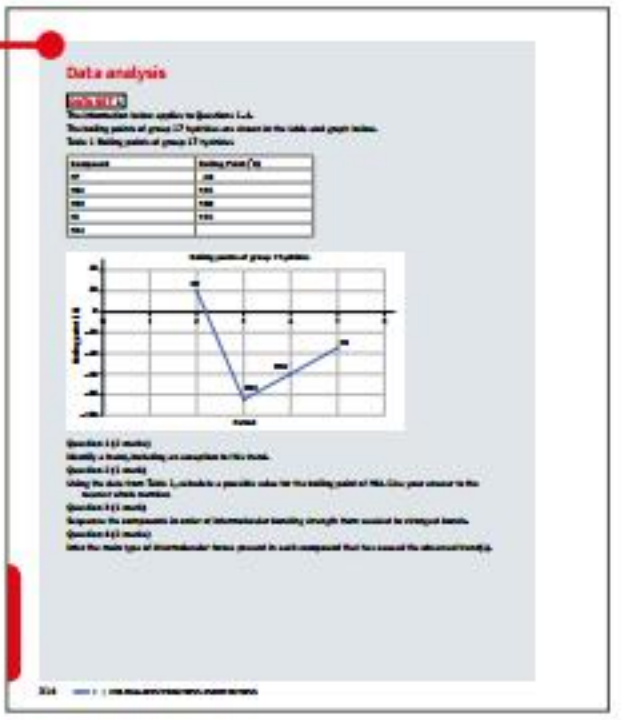
Each chapter finishes with a list of key terms covered in the chapter and a set of multiple choice and short response questions, reflecting the style and experience of the External Assessment (EA). These questions are organised under the four Assessment objectives for the subject matter: Describe, Apply, Analyse and Interpret.



How to use this book

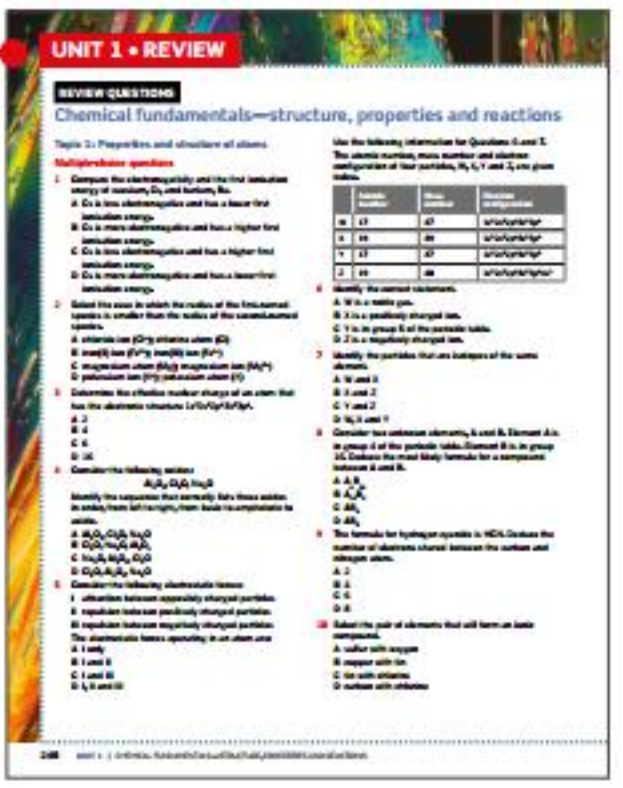
Data analysis

Data Analysis tasks at the end of each Chapter review provide an opportunity to respond to questions that use a range of qualitative and quantitative data relevant to that subject matter. The Data Analysis tasks are structured to reflect the approach taken in the Data Test IA1 and align with the Assessment objectives 2, 3 and 4.



Unit review

Each Unit finishes with a comprehensive set of exam-style instructions, including multiple choice and short response in the style of the External Assessment (EA). These review tasks assist students to draw together their science understanding subject matter of the whole unit.



Glossary

Key terms are shown in **bold** throughout the Student Book and are listed at the end of each chapter. A comprehensive glossary at the end of the book defines all the key terms. The glossary aligns with the syllabus context and includes the QCAA defined terminology.

Answers

Comprehensive answers and fully worked solutions for all Module review tasks, Try yourself, Science as a Human Endeavour, Chapter reviews and Unit reviews are provided via the eBook.

Icons

Go To icons make important links to relevant content within the student books in the course.

The Go To icons indicate:

- when a Practical Investigation would be suitable to engage with
- where support is available for skills and assessment tasks in Chapter 1 of your eBook.

Every Practical Investigation is supported by a complementary **SPARKlab** alternative practical.

Pearson

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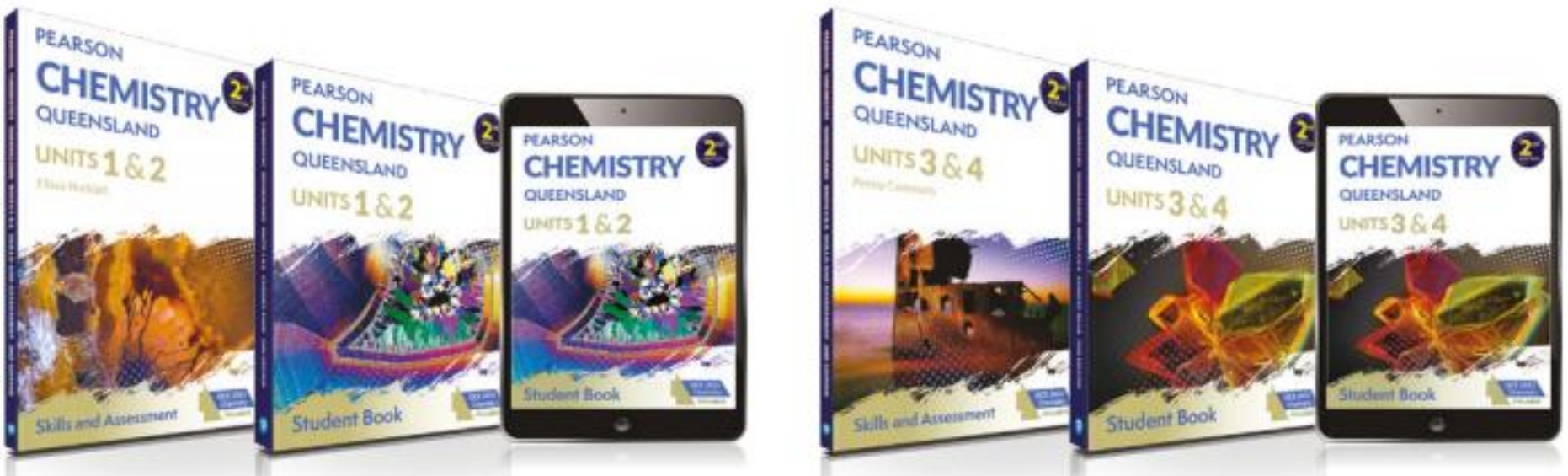
Trusted throughout Queensland to provide high quality support for implementation of the QCE Chemistry 2025 Syllabus, **Pearson Chemistry Queensland 2nd edition** has been refined to include what is needed to cover the QCE outcomes.



Student book

- The expert author team has delivered the same high-quality content you can trust, in the streamlined new edition for Queensland science classrooms.
- New, enhanced, and updated features that make the new second edition Student Books stand out:
  - New Science as a Human Endeavour sections
  - New Data Analysis tasks at the end of each Chapter review
  - Enhanced and updated Skills and Assessment Toolkit
  - Enhanced question sets
  - Updated Practical Manual of Practical Investigations
  - Updated Unit reviews and glossary.

Skills and assessment book

- The Skills and Assessment Book gives students the edge in preparing for all forms of assessment.
- It has been updated and refined to respond to the revised syllabus, and specifically provide opportunities to consolidate, develop and apply subject matter and Science inquiry skills. This resource features:
  - An updated Toolkit
  - Key knowledge summaries
  - Worksheets
  - Practical investigations and guidance
  - Assessment practice
  - Exam-style topic review sets.

eBook

Learner eBook access includes:

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CHAPTER

01 Chemistry skills and assessment toolkit

This chapter provides important information and support in the study of the QCAA Chemistry General Senior Syllabus for Units 1 to 4.

The Chemistry skills and assessment toolkit is designed to be used as a reference tool. It should be consulted on a need-to-know basis, where relevant, during this course of study. It is not intended that this chapter be worked through as a whole.

Focus

This chapter focuses on providing support and guidance in the following.

- **Development and application of scientific skills**
  - Mathematical and statistical processes used in chemistry
  - SI units
  - Visual representations
  - Graphical representations
  - Measurement errors and uncertainty
- **Completing the assessment tasks**
  - Data test
    - Preparation in skill development
  - Student experiment
    - Forming a relevant research question
    - Justifying experiment modifications
    - Developing a methodology
    - Finding sufficient, relevant data
    - Interpreting and analysing evidence
    - Evaluating experimental process
    - Scientific writing and representations
    - Referencing sources
  - Research investigation
    - Developing a research question from a claim
    - Collecting relevant and sufficient evidence to answer a research question
    - Identifying and analysing trends, patterns, relationships in the evidence
    - Evaluating the quality and limitations of the evidence
    - Evaluating the research process
    - Scientific writing and representations
    - Referencing sources

Assessment

In Units 1 and 2, students are required to complete at least two and no more than four assessment tasks developed by the teacher. At least one assessment task must be completed per Unit. In preparation for Chemistry Units 3 and 4, teachers may choose to mirror some of the assessment requirements of Units 3 and 4 in assessing Units 1 and 2.

The support material in this chapter is based on requirements in Units 3 and 4 and relates to the following assessments.

- Data test (Internal Assessment IA1)
- Student experiment (Internal Assessment IA2)
- Research investigation (Internal Assessment IA3)

Chapter organisation

The chapter is arranged in three parts:

- Part A: Working scientifically
- Part B: Student experiment
- Part C: Research investigation.

An outline of these parts is provided in the following pages.

QCAA Chemistry Syllabus objectives

- describe ideas and findings
- apply understanding
- analyse data
- interpret evidence
- evaluate conclusions, claims and processes
- investigate phenomena

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Part A: Working scientifically

Part A focuses on basic mathematical skills and their applications. It features many worked examples and opportunities to apply these examples yourself. These skills are assessed, directly and indirectly, in assessment tasks and by analysing data in practical investigations. Part A focuses on skills for the data test, and experiments. These skills are useful when completing sections of the student experiment, research investigation and the examination.

Refer to the following outline of Part A: Working scientifically to learn, revise and practise the skills in the areas in which you need help.

Module	Look here for	eBook page
1.1 Chemical science	- areas of chemistry - the work of scientific research	e6
1.2 Orders of magnitude	- scientific notation - transforming decimal notations to scientific notation - converting between scientific notation and scientific units, orders of magnitude and prefixes - SI prefixes - examples of calculations	e11
1.3 Mathematical basics for chemistry	- examples of maths used in chemistry - analysing straight line graphs	e17
1.4 Units	- measurement and units - correct use of unit symbols - SI units - unit conversions	e20
1.5 Measuring precision and accuracy using uncertainty and percentage error	- explanations of the terms: uncertainty, error, accuracy, precision - causes of errors - calculations with uncertainty and error bars - writing measurements with uncertainty and error values - writing measurements and calculations to the correct significant figure - determining the absolute uncertainty of a value - converting between absolute and percentage uncertainties - calculating a value along with the associated uncertainty - calculating percentage error	e23
1.6 Tables and graphing	- arranging and recording data in tables - converting data from tables to graphs - types of graphs—scatterplots, line graphs, bar and column graphs - outliers and how they are represented on graphs - representing missing data on graphs	e40
1.7 Data analysis	- calculating mean, median, mode, range - regression, linear regression, and coefficient of determination	e48
1.8 Scientific writing	- writing scientifically - developing scientific representations - maintaining a science journal - referencing sources - in-text citations - using AI in research and writing - plagiarism - referencing AI sources - multimodal presentations	e52

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Part B: Student experiment

Part B focuses on the student experiment. This internal assessment task requires students to follow the full scientific method over an extended and defined period of time. Students develop their own research question to investigate, based on an identified experiment related to Unit 3 subject matter.

Part B supports you through all aspects of the student experiment. The QCAA objectives and instrument-specific marking guide (ISMG) for the assessment are explained.

Part B provides examples of how to **modify** (**extend**, **refine** or **redirect)** the initial experiment to write an experimental research question. Included is a step-by-step guide to evaluate the quality of your question and explanations of scientific methodology. Part B also covers data types, data collection and analysis of data to draw valid conclusions. It includes how to evaluate the quality of data, including its reliability and validity, and how to link these to improvements and extensions. Also provided is support in writing up your scientific report, covering writing conventions and referencing sources.

Refer to the following outline of Part B: Student experiment to learn, revise and practise your skills in the areas in which you need help.

Module	Look here for	eBook page
1.9 Forming	- establishing background information - developing a rationale - defining variables - developing the research question - evaluating the research question - justifying the question modification - putting it all together: sample report	e65
1.10 Finding	- determining the risk assessment - managing risk - considering environmental and ethical issues - collecting sufficient and relevant raw data - collecting data electronically - putting it all together: sample report	e76
1.11 Analysing	- presenting the data - processing data using mathematical techniques - identifying patterns, relationships, trends in data - interpreting results - identifying uncertainty and limitations in the evidence - putting it all together: sample report	e86
1.12 Interpreting and evaluating	- drawing a conclusion that is linked to research question - discussing reliability and validity - identify improvements and extensions to the research - putting it all together: sample report	e91

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Part C: Research investigation

Part C focuses on the research investigation. This internal assessment task requires students to gather secondary evidence on a research question. It is completed over an extended and defined period of time. Students develop their own research question to investigate, based on a claim related to Unit 4 subject matter.

Part C supports you through all aspects of the research investigation. The QCAA objectives and instrument-specific marking guide (ISMG) for the assessment are explained.

Part C assists with writing your research question. It considers examples of claims and how to analyse claims for context, and guides you in developing your own research question. You will be guided in writing a specific and relevant research question that encompasses a small sub-section of the claim and is linked to Chemistry syllabus concepts. You will consider the information on locating and evaluating suitable secondary sources for the research, including identifying errors and relationships in data and assessing validity. You will learn how to formulate a justified conclusion and describe improvements and extensions. There is support for writing your scientific report including scientific writing style and the structure of the report.

Refer to the following outline of Part C: Research investigation to learn, revise and practise your skills in the areas in which you need help.

Module	Look here for	eBook page
1.13 Forming and finding	- understanding a claim - classifying elements in the claim - identifying variables, terms and concepts related to the claim - developing a research question - planning the research - refining a research question - locating sources - putting it all together: sample report	e97
1.14 Analysing	- collecting sufficient and relevant evidence - identifying trends, patterns, relationships in the evidence - assessing limitations of the evidence - putting it all together: sample report	e110
1.15 Interpreting	- assessing if the evidence justifies the claim - presenting an argument on whether the claim is justified - reaching a conclusion about the claim - putting it all together: sample report	e116
1.16 Evaluating	- evaluating the quality of the evidence - suggesting any extrapolations of the claim - suggesting any improvements/extensions to the investigation - putting it all together: sample report	e119

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1.1 Chemical science

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that chemistry is the study of materials and their properties and structure
- appreciate that chemistry uses mathematics
- explain the difference between scientific models, theories, laws, principles and facts
- understand that chemistry uses natural laws, theories, models and principles to describe real phenomena
- appreciate that understanding the theories and models that describe and explain the structure and properties of chemicals will help you make predictions and understand chemical systems
- recall the major areas of chemistry
- explain how a vast number of professions use some aspect of chemistry
- appreciate that chemistry is a dynamic and evolving branch of science and helps to explain phenomena and solve problems encountered in an ever-changing world
- understand that science provides a systematic approach for comprehending the world.

Science is a human endeavour to understand the world and the known universe. It is one method of many used to develop knowledge. This knowledge is continually refined and redefined. Science follows a **methodology** to observe, test, measure, analyse and evaluate natural **phenomena** in a way that humans can understand and that allows us to construct meaning. There is no single **scientific method**; however, science follows a cyclical process including observation of natural phenomena, questioning, hypothesising and predicting, experimentation and gathering **data**, refining and altering all previous elements, and theorising (Figure 1.1.1).

In the Chemistry course, you will develop an understanding of chemical systems, and how **models** of matter and energy transfers and transformations can be used to describe, explain and predict chemical structures, properties and reactions.

FIGURE 1.1.1 A schematic outlining the processes involved in the scientific method. The scientific method is more of a cyclical process rather than linear.

Today, all scientific disciplines are expanding into new frontiers. The number of divisions and fields in chemistry is ever-increasing, and the relationship between disciplines is becoming more intertwined.

Innovations today are crossing traditional barriers between technology, chemistry, physics and biology of the past 100 or so years.

AREAS OF CHEMISTRY

Chemistry has been traditionally divided into four major areas—organic, inorganic analytical and physical chemistry.

Organic chemistry deals with molecules formed predominantly from carbon, hydrogen, oxygen and nitrogen. The range and diversity of organic molecules is enormous—literally millions of molecules have been identified. Very long molecules can be made up of much smaller organic building blocks, forming polymers such as the plastics that have become so common over the past few decades. Because living organisms are made up primarily of organic molecules, organic chemistry forms the molecular foundation of the biological sciences and is intimately linked with pharmaceuticals and drug design.

Inorganic chemistry is the study of molecules composed of other elements and includes salts, metals, semiconductors and nanomaterials. Biologically important molecules such as vitamins, haemoglobin and chlorophyll contain metal atoms and organic sections.

Inorganic and organic chemistry often involve the design and synthesis of new materials with particular chemical and physical properties related to chemical reactivity, boiling point, strength, colour or magnetism.

Analytical chemistry involves the analysis and quantification of chemical components of a sample. This is increasingly important with regards to the quality of manufactured goods, and in monitoring pollutant concentrations in our air, water and food. Even very low amounts of substances such as mercury or dioxins can be harmful to human health or the environment. Therefore, detecting and quantifying the amounts of these pollutants presents an ongoing intellectual and technical challenge.

Physical chemistry is the area of study of the physical properties, energies and spectra of all types of molecules, and the rate of chemical reactions. Physical chemists typically use spectroscopic or computational methods to study molecules, surfaces and chemical reactions. Sophisticated experimental techniques are required to probe complex or fast chemical processes, such as those that occur during combustion or the reactions taking place in the atmosphere.

Although traditional divisions in chemistry are still of vital importance, most of the exciting current scientific research is interdisciplinary and involves collaboration with many other scientific and technical fields including physics, biology, pharmacology, materials science, environmental science and engineering, leading to developments in nanotechnology, materials, pharmaceutical chemistry and environmental research.

The role and work of a chemist

Those who study chemistry are typically known as chemists. However, as the world is changing, science, technology, engineering and maths (STEM) fields are integrating numerous disciplines into vocational roles. A recent report from a multinational business organisation indicates that jobs in as much as 75% of growing and future industries will require STEM qualifications.

A STEM qualification fosters skills in areas such as creativity and critical thinking, and is highly regarded in public and private businesses. According to this report, the safest future occupations are doctors, nurses and teachers. The Australian Government's chief scientist report states that of Australia's current STEM workforce, only 3.3% of STEM students graduated with a major in chemical sciences. There are numerous reports every year outlining that the majority of future professions will be STEM related.

The advances in scientific endeavours as well as innovations have seen a significant increase in multiple scientific specialities and disciplines working together. When more than one discipline is required to solve a problem or develop an innovation, it is said to be transdisciplinary. Transdisciplinary approaches to scientific endeavours form the heart of STEM.

The Royal Australian Chemical Institute identifies the jobs shown in Table 1.1.1 as being directly related to a chemistry qualification, but there are many other jobs for which chemistry is a useful background subject.

TABLE 1.1.1 Jobs in chemistry

Job	Typical job description
analytical chemist	uses a diverse range of methods to investigate the chemical nature of substances, to identify and understand the substance and to determine how it behaves in different conditions
clinical biochemist	analyses and interprets data relating to patients' samples to assist with the investigation, diagnosis and treatment of diseases
forensic scientist	provides impartial scientific evidence for use in courts of law to support the prosecution or defence in criminal and civil investigations
research scientist (physical sciences)	studies non-living systems to increase our understanding of how the physical world works; disciplines include astronomy, chemistry, earth science, materials science, meteorology and physics
chemical development engineer	involved in the development of industrial processes for the production of a diverse range of products, as well as in commodity and specialty chemicals
science writer	researches, writes and edits scientific news articles and features for business, trade and professional publications, specialist scientific and technical journals, and the general media
toxicologist	plans and carries out laboratory and field studies to identify, monitor and evaluate the impact of toxic materials and radiation on human and animal health, the environment, and the impact of future technology
process engineer	develops economical industrial processes to make the huge range of products on which modern society depends, including food and drink, fuel, artificial fibres, pharmaceuticals, chemicals, plastics, toiletries, energy and clean water

Table 1.1.2 lists jobs where a chemistry degree would be useful.

TABLE 1.1.2 A degree in chemistry would be beneficial in these jobs

Job	Typical role description
patent agent	A patent agent obtains and enforces intellectual property rights on behalf of either individual inventors or organisations. Patents are granted by the government and give inventors the right to prevent the commercial use of inventions by other parties for a limited period. Chemists can specialise in pharmaceutical patent law.
environmental consultant	An environmental consultant works on commercial or government contracts to address a variety of environmental issues for their clients. This work covers a wide range of disciplines such as assessment of air, land and water contamination, environmental impact assessment, environmental audit, waste management, and the development of environmental policy and environmental management systems.
secondary school teacher or university lecturer	In addition to teaching chemistry to students, lecturers, in particular, may also undertake academic or industry research and may be involved in school or departmental management.

A list of some of the careers related to chemistry can be seen in Figure 1.1.2. The levels shown indicate the amount of training required, with Level 4 being the highest.

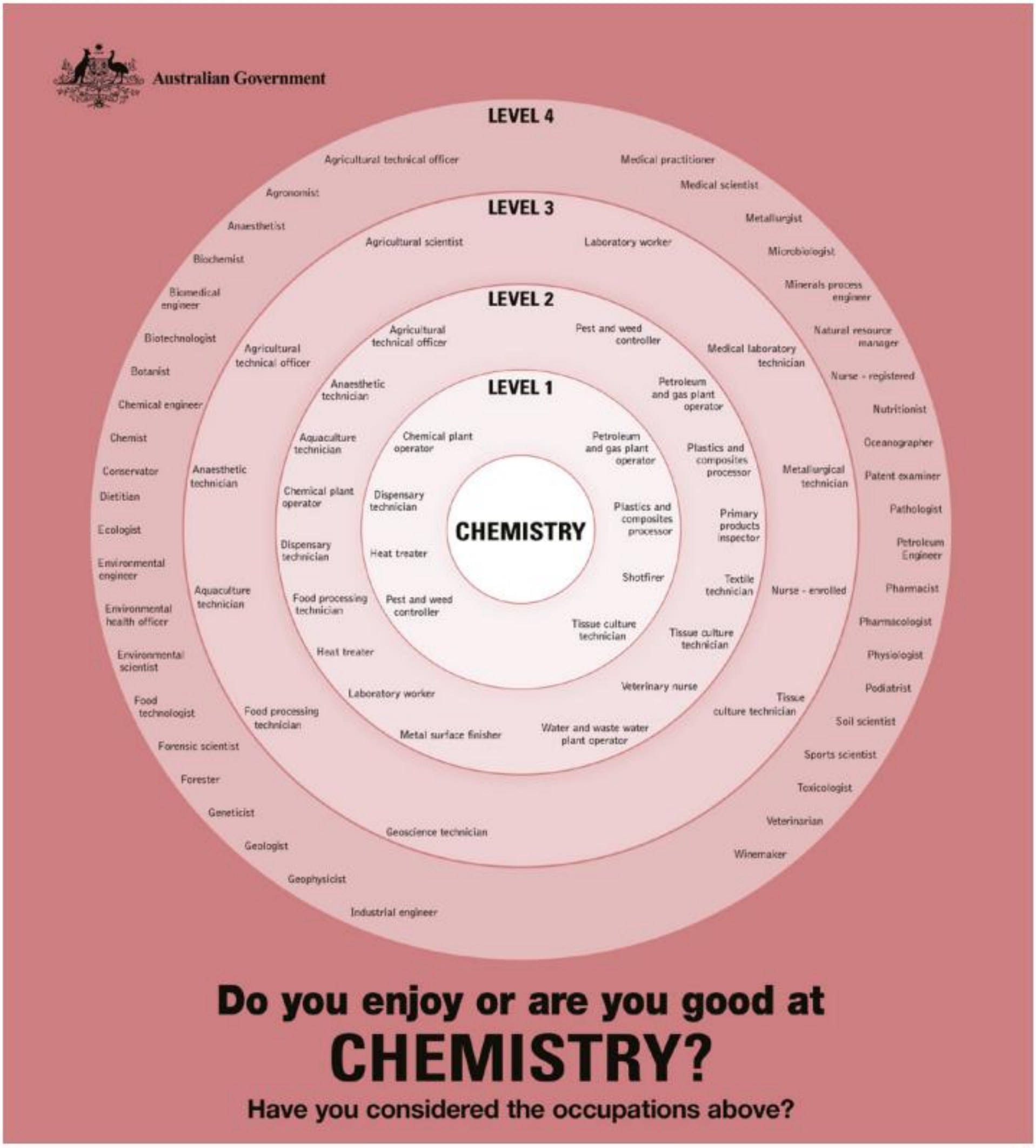


FIGURE 1.1.2 Examples of careers in fields related to chemistry.

THE WORK OF SCIENTIFIC RESEARCH

The foundation of all sciences, including chemistry, is scientific research. Scientific research works in the unknown to develop new understandings. To build evidence, it may take years and many experiments. In interpreting scientific evidence, scientists endeavour to establish models, **theories**, **laws**, **principles** and facts. These change over time as knowledge develops, as illustrated in Figure 1.1.3.

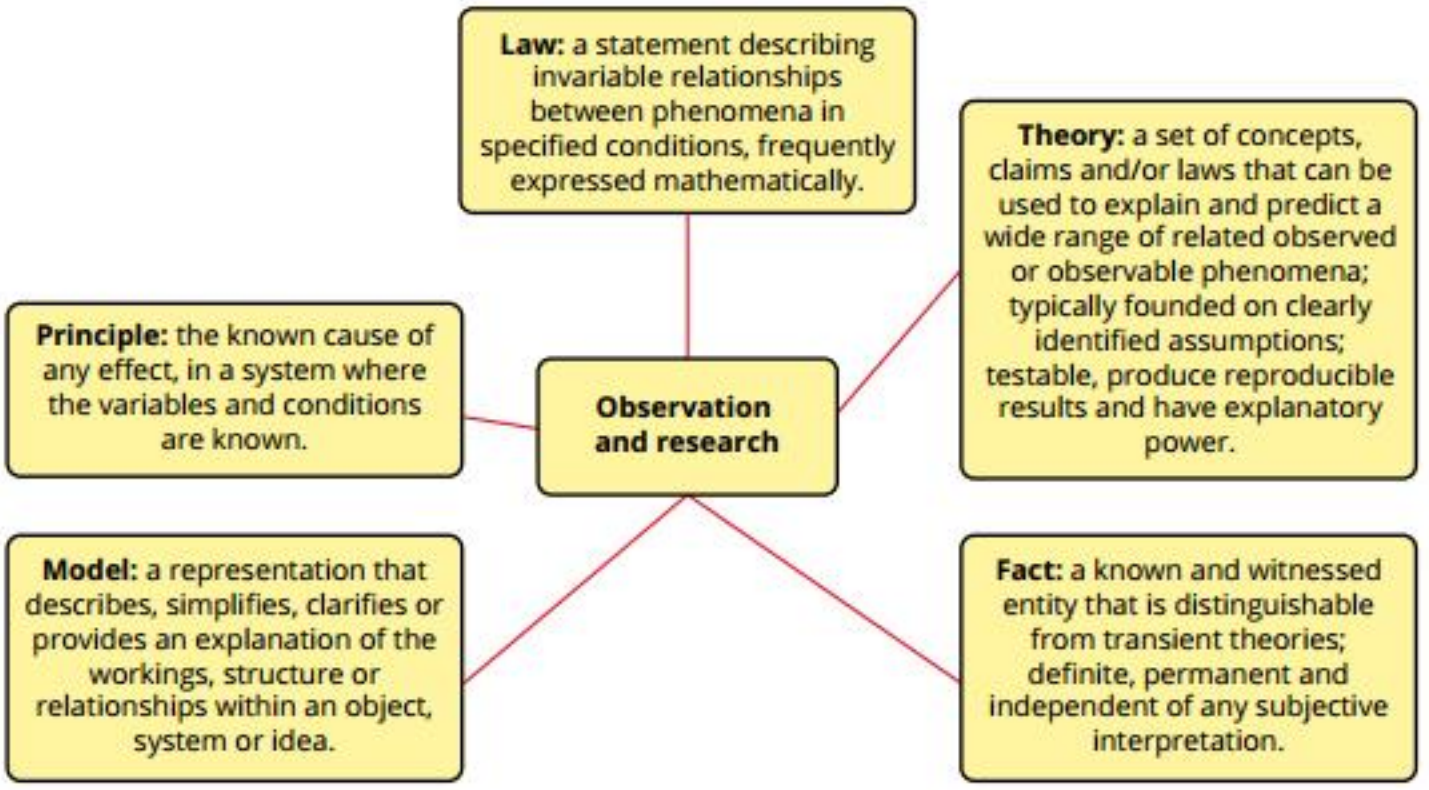

Law: a statement describing invariable relationships between phenomena in specified conditions, frequently expressed mathematically.
Theory: a set of concepts, claims and/or laws that can be used to explain and predict a wide range of related observed or observable phenomena; typically founded on clearly identified assumptions; testable, produce reproducible results and have explanatory power.
Principle: the known cause of any effect, in a system where the variables and conditions are known.
Observation and research
Model: a representation that describes, simplifies, clarifies or provides an explanation of the workings, structure or relationships within an object, system or idea.
Fact: a known and witnessed entity that is distinguishable from transient theories; definite, permanent and independent of any subjective interpretation.

FIGURE 1.1.3 Scientific research and observations are used to establish or develop models, principles, laws, theories and facts.

1.1 Review

SUMMARY

- Science is known as a systematic approach to develop knowledge through testable explanations and repeatable means.
- Chemistry is the study of chemical systems, and how models of matter, energy transfer and transformations can be used to describe, explain and predict chemical reactions.
- There are four main areas of chemistry: organic, inorganic, physical and analytical.
- STEM (science, technology, engineering and mathematics) research is a transdisciplinary approach to scientific endeavours.
- Scientific evidence is used to formulate and establish models, theories, laws, principles and facts.
- A scientific model is a representation of a process, a phenomenon or data.
- A scientific theory is a well-established understanding and conceptual explanation of phenomena based on a body of evidence.
- A scientific law is a statement that describes relationships between phenomena in specified conditions.
- A scientific principle is the known cause of any effect in a system where the variables and conditions are known.
- A scientific fact is something that is known and witnessed and is distinguishable from transient theories; facts are definite, permanent and independent of any subjective interpretation.

Part A will consider the basic mathematical and data skills and applications that will be required for the student experiment, research investigation, data test and practicals.

1.2 Orders of magnitude

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- convert numbers to and from scientific notation
- estimate the value of a quantity using its order of magnitude
- recognise common SI prefixes.

SCIENTIFIC NOTATION

In scientific research and literature, measurements are often written in **scientific notation** to overcome confusion or ambiguity when displaying numbers with magnitude; for example 2.56×10^{-6}. It is important to understand the numbers in scientific notation, their order of magnitude and how to convert them into other units.

Quantities are written as a number between one and ten, and then multiplied by an appropriate power of ten. Note that 'scientific notation', 'standard notation', 'standard form' and 'power of ten notation' all have the same meaning.

SKILLBUILDER 1.2.1

Transforming decimal notation to scientific notation

Scientists use scientific notation to handle very large and very small numbers. For example, instead of writing 0.000000035, scientists would write 3.5×10^{-8}.

A number in scientific notation is written as:

$a \times 10^n$

where:

- a is called the coefficient, and is a real number between 1 and 10; that is $1 \leq a < 10$
- n is called the exponent, and is an integer (a positive or negative whole number). n is the power that 10 is raised to.

Note that if n is positive, then the number is larger than one, and if n is negative, then the number is less than 1.

To transform a very large or very small number into scientific notation, perform these steps.

1. Move the decimal place from its position in the original number until you get a number that is greater than or equal to 1 but less than 10.
2. Count the number of places that the decimal point has moved. This number is the exponent—the power of ten (Figure 1.2.1).

- If the decimal point is moved n places to the left, n will be a positive number; for example, $510 = 5.1 \times 10^2$.
- If the decimal point is moved n places to the right, n will be a negative number; for example, $0.051 = 5.1 \times 10^{-2}$.

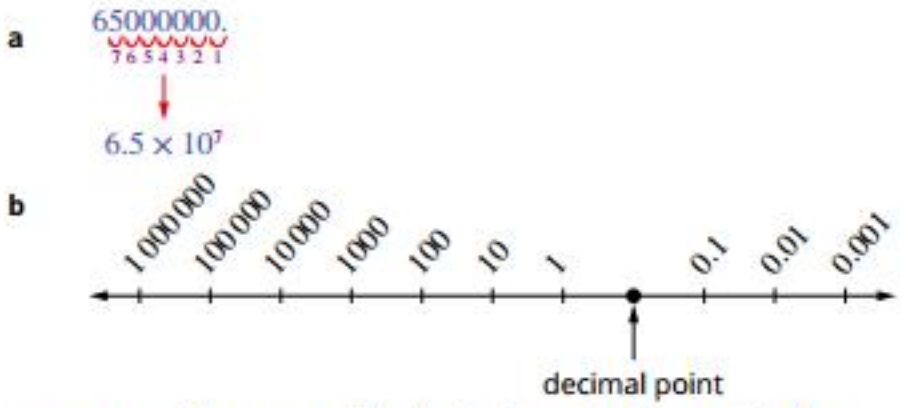


FIGURE 1.2.1 The exponential value is determined by counting the number of places the decimal point needs to be moved.

TABLE 1.2.1 Converting from scientific notation

Scientific notation	Number (expanded form)
1×10^{-9}	0.000000001
1×10^{-6}	0.000001
1×10^{-3}	0.001
1×10^{-1}	0.1
1	1
1×10^{1}	10
1×10^{3}	1000
1×10^{6}	1000000
1×10^{9}	1000000000

You will notice from Table 1.2.1 that when large numbers are written in scientific notation, the 10 has a positive exponential value. Very small numbers smaller than 1 are written with 10 to a negative exponent.

Test the skill

Convert 121000 to scientific notation.

Examples of some values written in scientific notation are:

6.02×10^{23} particles

$25.25\,\text{mL} = 2.525 \times 10^{-2}\,\text{L}$

$0.00302\,\text{mol} = 3.02 \times 10^{-3}\,\text{mol}$

Values given in scientific notation show the significant numbers and indicate the precision of measurement during experimentation by the instrument. Precision and accuracy are covered in more detail in Module 1.5.

Worked example 1.2.1

CONVERTING TO SCIENTIFIC NOTATION

The radius of a sodium atom is 0.000 000 000 160 m. How many individual sodium atoms can fit across a typical pin head with a diameter of 1.5 mm?	
Thinking	**Working**
Calculate the diameter of a sodium atom (twice the radius).	0.000 000 000 320 m
Convert to scientific notation.	
Move the decimal place so that the number is represented as a number between 1 and 10.	0.000 000 000 320 → 3.20
Count the number of places the decimal place was moved.	10
Use the number of decimal places moved as the power exponent to base 10.	3.20×10^{10}
Determine whether the decimal was moved left or right.	right
Place a negative symbol (–) in front of the power of 10.	$3.20 \times 10^{-10}\,\text{m}$
Convert 1.5 mm to m.	1.5 mm = 0.15 cm = 0.0015 m
Convert to scientific notation using the same steps as above.	$1.5 \times 10^{-3}\,\text{m}$
Now calculate the number of individual sodium atoms that can fit on a pin head by dividing the pin head diameter (1.5×10^{-3} m) by the sodium atom diameter (3.20×10^{-10} m).	$\text{number} = \frac{1.5 \times 10^{-3}}{3.20 \times 10^{-10}} = 4.7 \times 10^{6}$

➤ Try yourself 1.2.1

CONVERTING TO SCIENTIFIC NOTATION

The radius of a chloride ion is 0.000 000 000 181 m. Calculate how many chloride ions could fit across a pin head with a diameter of 1.5 mm.

You should be routinely using scientific notation to express very large and very small numbers. This also involves learning to use your calculator intelligently. Scientific and graphics calculators can be put into a mode whereby all numbers are displayed in scientific notation. It is useful when doing calculations to use this mode rather than frequently attempting to convert to scientific notation by counting digits on the calculator display.

An important reason for using scientific notation is that it removes ambiguity about the precision of some measurements. For example, a measurement recorded as 240 g could be a measurement to the nearest gram; that is, somewhere between 239.5 g and 240.5 g, or it could have been rounded up to the nearest 10 g. Writing this quantity as 2.40×10^{2} g makes the accuracy of the value clear (in this case, 3 significant figures).

Writing numbers using scientific notation

To write a number into long form from scientific notation, follow these rules.

- If the exponent is positive, write the coefficient without the decimal point. Continue to write zeros after the last digit in the coefficient until the number of digits after the first digit is equal to the exponent.
- If the exponent is negative, write a zero in the ones place value holder, then a decimal point. Continue to write zeros until the total number of zeros (including the zero in the ones place value holder) is equal to the positive value of the exponent. Then write the coefficient without the decimal place.

Worked example 1.2.2

WRITING QUANTITIES FROM SCIENTIFIC NOTATION

The mass of a neutron is 1.675×10^{-27} kg. Write this value in long form.

Thinking	Working
The exponent is negative, which means the number in long form is less than 1. Write a zero in the ones column and then a decimal point. After the decimal point, write another 26 zeros followed by the coefficient without the decimal place.	0.00000000000000000000000001675 kg

➤ Try yourself 1.2.2

WRITING QUANTITIES FROM SCIENTIFIC NOTATION

Write the following values in long form.

a the diameter of a magnesium ion is 1.44×10^{-10} m

b the number of hydrogen molecules in 1 mole of hydrogen gas is 6.02×10^{23}

Scientific notation is the preferred way of communicating very large and very small numbers (such as measurements) in chemistry. Often for convenience and ease of use, quantities in chemistry problems should first be converted into scientific notation before any calculations can be carried out.

ORDERS OF MAGNITUDE AND PREFIXES

As stated above, scientists often work with very large or very small numbers in the measurements made during experimentation. These can be written using scientific notation or using a prefix before the unit to represent the order of magnitude. For example, a measurement of 2.56×10^{-6} m can be written as 256 μm. The symbol μ represents the prefix *micro* (Table 1.2.2), which means 'one millionth of the measured unit'. So, when *micro* is placed in front of metre, it becomes micrometre, meaning 'one millionth of a metre', therefore 256 μm becomes 256 millionths of a metre. An International System of units (SI) **prefix** is a symbol written at the front of a unit to indicate that the measurement is a power of ten higher or lower than the unit itself.

There are twenty SI prefixes in use and most of them denote units that are one thousand (10^3) times larger or smaller than the previous prefix. Table 1.2.2 lists the SI prefixes commonly used in chemistry. You should become familiar with both scientific notation and prefixes for units of measurement. You should also be able to use them interchangeably.

TABLE 1.2.2 Common SI prefixes used in chemistry

Prefix	Symbol	Multiplier	Description	Decimal	Example
tera	T	10^{12}	trillion	1 000 000 000 000	Electricity generation provides over 20 000 terawatt-hours of energy a year.
giga	G	10^{9}	billion	1 000 000 000	Over 10 gigatonnes of carbon dioxide is produced from burning coal.
mega	M	10^{6}	million	1 000 000	1 MHz is close to the frequencies at which TV stations broadcast.
kilo	k	10^{3}	thousand	1000	1 kg is 1000 g.
hecto	h	10^{2}	hundred	100	1 hPa is a unit used in meteorology used to describe atmospheric pressure.
–	–	1	unit	1	–
deci	d	10^{-1}	tenth	0.1	A cube that holds 1 L has a capacity of 1 dm^3 (one cubic decimetre).
centi	c	10^{-2}	hundredth	0.01	1 cm is the same as 1/100th of a metre or 0.01 m.
milli	m	10^{-3}	thousandth	0.001	There are 1000 mm in 1 m.
micro	μ	10^{-6}	millionth	0.000 001	μg is commonly used as the unit for medicine dosage.
nano	n	10^{-9}	billionth	0.000 000 001	The wavelength of yellow sodium streetlights is 550 nm.
pico	p	10^{-12}	trillionth	0.000 000 000 001	The diameter of the hydrogen atom is about 100 pm.
femto	f	10^{-15}	quadrillionth	0.000 000 000 000 001	Some lasers emit a pulse of light that lasts for 1 fs.

i SI prefixes are used to avoid writing very small or very large numbers with lots of zeros. The prefix is added directly to the name of a unit, and a prefix symbol attaches directly to the symbol for a unit.

Do not put spaces between the prefixes and the unit symbols. The larger prefixes are written as a capital letter, while the smaller prefixes are written using a lower case letter. It is important to give a symbol the correct case (upper or lower case). There is a big difference between 1 mm and 1 Mm!

Note that the fundamental unit kilogram contains a prefix, but all multiples of mass are written with the base unit grams. As an example, one million kilograms is not written as one megakilogram but as one gigagram (Gg).

Before any measurements with a prefix can be substituted into a formula, they must be converted into SI units without the prefix, i.e. written in scientific notation.

SKILLBUILDER 1.2.2

Converting between units

Often, in science, you may need to convert from one unit to another to complete a calculation. Knowing how to change between units is an important skill; however, conversion factors should be used carefully. As some units of measurement are difficult to visualise, knowing the size of different units in relation to each other will aid your understanding and help you avoid errors in your calculations. The most common mistake made with conversion factors is multiplying rather than dividing.

Cortisol is a natural hormone found in the body; however, it is used by some athletes to increase performance. Normal levels of cortisol in the blood are around 400 $nmol\,L^{-1}$. To put this into context, you can convert this value into a unit you can easily visualise, like grams per litre ($g\,L^{-1}$).

To convert 400 $nmol\,L^{-1}$ to $mol\,L^{-1}$ (before converting to $g\,L^{-1}$), you need to move the decimal nine places to the left, so it becomes 0.000 000 4 $mol\,L^{-1}$.

This can also be written as $4.0 \times 10^{-7}\,mol\,L^{-1}$.

One mole of cortisol weighs 362.46 g, therefore 0.000 000 4 $mol\,L^{-1}$ is equal to 0.000 145 $g\,L^{-1}$ (or $1.45 \times 10^{-4}\,g\,L^{-1}$)—very small indeed!

Worked example 1.2.3

CONVERTING BETWEEN UNITS

Convert 60 700 grams to kilograms.	
Thinking	**Working**
Consider the units from grams to kilograms.	$= \frac{g}{} \times \frac{kg}{g}$ $= \frac{\cancel{g}}{} \times \frac{kg}{\cancel{g}}$ $= kg$
To convert grams to kilograms, multiply 60 700 by kg per g. Since 1 kg = 1000 g, the kg is replaced by 1 and the g is replaced by 1000.	$= \frac{60\,700}{} \times \frac{kg}{g}$ $= \frac{60\,700}{} \times \frac{1}{1000}$ $= 60.7\,kg$

➤ Try yourself 1.2.3

CONVERTING BETWEEN UNITS

The rate of combustion of propane has been determined by measuring the production of CO_2 in mL. If CO_2 was generated at a rate of 25 $\mu L s^{-1}$, determine what this rate is in $mL s^{-1}$. Calculate how many litres of CO_2 would be produced in one hour.

When converting from one unit to another it is essential that you check that the answer makes sense. For instance, if converting from μm to km, you would expect that there are many μm in a km. The inversion of prefix conversions is one of the major sources of mistakes in general chemistry.

1.2 Review

SUMMARY

- 'Scientific notation', 'standard notation', 'standard form' and 'power of ten notation' all have the same meaning.
- A number in scientific notation is written as $a \times 10^n$, where:
  - a is called the coefficient, and is a real number between 1 and 10; that is, $1 \leq a < 10$
  - n is called the exponent, and is an integer (positive or negative).
- Prefixes are written in front of units to represent orders of magnitude.
- When converting units, it can be useful to write the conversions as fractions and then cross-cancel out to ensure that the conversion is done correctly.

KEY QUESTIONS

Describe

1 State why chemists need to write numbers in scientific notation instead of long form.

2 Identify the two numbers between which the coefficient of a number expressed in scientific notation has to lie.

3 State what the unit Tg means.

Apply

4 Represent the following values in scientific notation.

a 637 nm, expressed in m

b 319 s, expressed in s

5 Represent the following numbers in long form.

a 1.1×10^{-10} m

b 7.031×10^{6} m s^{-2}

6 Match each number with its scientific notation.

Number	Scientific notation
0.002	2×10^{3}
2000	1.234×10^{-1}
0.1234	2×10^{-3}
123.4	1.234×10^{1}
12.34	1.234×10^{2}

Analyse

7 Convert the following lengths into the unit in brackets, presenting the information in scientific notation.

a 1.56 mm (μm)

b 8.35 nm (cm)

8 A human hair is about 50 μm wide, whereas a virus is 2×10^{-8} m wide. How many times wider than the width of the virus is the width of the human hair?

1.3 Mathematical basics for chemistry

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that the rules of mathematics apply for solving mathematical operations or calculations in chemistry
- perform basic mathematical operations using percentages and fractions
- rearrange and substitute formulas using algebraic rules
- use the equation of a straight line to determine its gradient and *y*-intercept.

Science uses mathematics in working with data. The evidence can be quantified, measured and analysed. This is known as statistical analysis (a branch of mathematics).

When conducting mathematical operations or calculations, remember that all the rules of mathematics apply, including:

- order of operations
- rules for transposing formulas and working with fractions
- substitutions
- approximations.

EXAMPLES OF MATHEMATICAL BASICS FOR CHEMISTRY

Worked example 1.3.1 demonstrates examples of mathematics in chemistry.

Worked example 1.3.1

MATHEMATICAL BASICS IN CHEMISTRY

The rate of the reaction between two chemicals is given by the expression:
rate = $k[A][B]$
where k is the rate constant.
Determine the rate when $k = 2.503\ (\text{mol dm}^{-3})^{-1}\text{s}^{-1}$, $[A] = 0.100\ \text{mmol L}^{-1}$ and $[B] = 180.0\ \mu\text{mol dm}^{-3}$.

Thinking	Working
Convert the units and prefixes into SI units and scientific notation (if required).	$[A] = 1.00 \times 10^{-4}\ \text{mol dm}^{-3}$ $[B] = 180.0 \times 10^{-6}\ \text{mol dm}^{-3}$ (or $1.800 \times 10^{-4}\ \text{mol dm}^{-3}$)
Write down the equation.	rate = $k[A][B]$
Substitute in the values.	rate = $2.503 \times 10^{-3} \times 1.00 \times 10^{-4} \times 1.800 \times 10^{-4}$ $= 4.5054 \times 10^{-11}\ \text{mol dm}^{-3}\text{s}^{-1}$
Express to the lowest number of significant figures in the data.	rate = $4.51 \times 10^{-11}\ \text{mol dm}^{-3}\text{s}^{-1}$

➤ Try yourself 1.3.1

MATHEMATICAL BASICS IN CHEMISTRY

A hydrogen atom has a diameter of 64 pm. If the atom is represented as a sphere, calculate:

a the volume of a hydrogen atom

b the surface area of a hydrogen atom.

ANALYSING STRAIGHT LINES

A straight line is the simplest relationship between two variables. The **dependent variable** is plotted on the *y*-axis and the **independent variable** is on the *x*-axis. The relationship between the two variables is represented by the gradient. Figure 1.3.1 shows a typical straight line relationship.

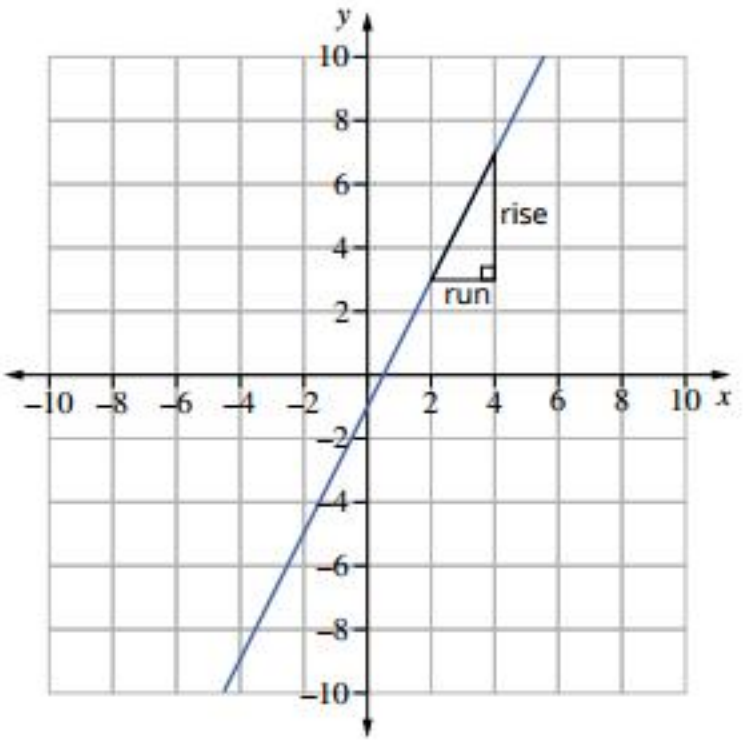


FIGURE 1.3.1 A graph representing a simple relationship between two variables.

The *y*-intercept and gradient can be easily calculated by hand or with technology. The gradient of any straight line is calculated using:

$$\text{gradient, } m = \frac{\text{rise}}{\text{run}} = \frac{\Delta y}{\Delta x}$$

The *y*-intercept, *c*, is read off the *y*-axis.

The equation of any straight line is determined by the gradient and *y*-intercept:

$$y = mx + c$$

In the example in Figure 1.3.1, the equation of the straight line is $y = 2x - 1$ with a gradient of 2 and *y*-intercept of −1.

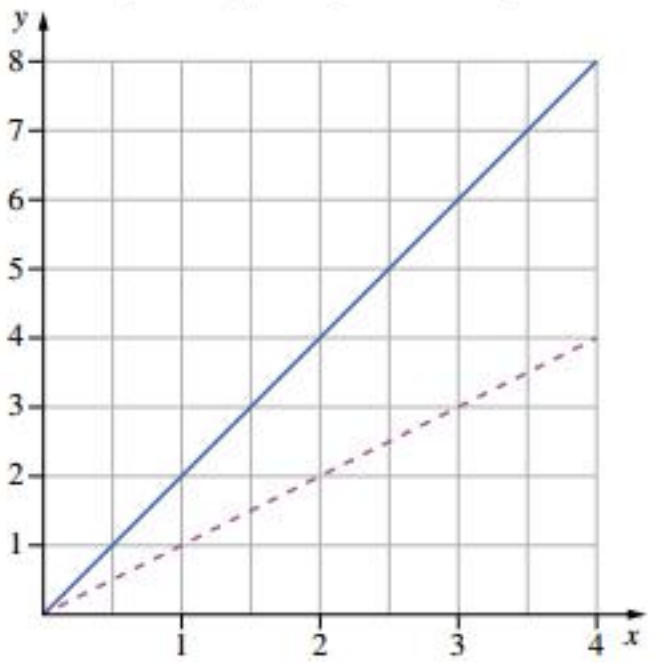
SKILLBUILDER 1.3.1

Interpreting the slope of a linear graph

Scientists often represent a relationship between two variables as a graph. For directly proportional relationships, the variables are related to each other by a straight line, where the slope (or gradient) of the line represents the constant of proportionality between the two variables.

The slope or gradient of the line is defined as the ratio of change between two points in the vertical axis (Δy), divided by the change between two points in the horizontal axis (Δx). In other words, it measures the rate at which one variable (the dependent variable) changes with respect to the other (the independent variable).

The slope of a linear graph indicates the rate of change of the dependent variable (*y*-axis) with respect to the independent variable (*x*-axis). The graph on the right has two straight lines with different slopes. The steeper slope (solid line) indicates that the rate of change is higher. This means the change is happening more quickly. On the other hand, the flatter slope (dashed line) indicates that the rate of change is lower. This means the change is happening more slowly.



Worked example 1.3.2

INTERPRETING THE SLOPE OF A LINEAR GRAPH

On a graph with two sloped lines, identify what the steeper sloped line indicates.

A a faster rate of change
B a slower rate of change
C the same rate of change
D a much slower rate of change

Thinking	Working
The slope or gradient of the line is defined as the ratio of change between two points in the vertical axis (Δy), divided by the change between two points in the horizontal axis (Δx).	A is correct. The steepness of the slope indicates the rate of change. A line with a steeper slope indicates a faster rate of change.

➤ Try yourself 1.3.2

INTERPRETING THE SLOPE OF A LINEAR GRAPH

Identify which of the following options indicates the rate of change of a straight line on a graph.

A area under the graph
B *y*-intercept
C *x*-intercept
D gradient

1.3 Review

SUMMARY

- When conducting mathematical operations or calculations, remember that all the rules of mathematics apply, including:
  - order of operations
  - rules for transposing formulas and working with fractions
  - substitutions
  - approximations.

KEY QUESTIONS

Describe

1 State the formula for calculating the gradient of a straight line.

Apply

2 Determine these quantities.

a the mass of 75 mL of ethanol (density of ethanol is $0.789\,g\,mL^{-1}$)
b the volume of 24.5 g of ethanol

Analyse

3 A student recorded the following temperatures of water.

Time (min)	Temperature (°C)
0	22
2	34
4	43
5	50
8	64
10	78

a Calculate the average temperature change per minute during the experiment.
b Determine whether the increase was constant throughout the experiment.

1.4 Units

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- appreciate that chemistry uses the International System (SI) of units
- recall fundamental units, their symbols and definitions
- convert between various units of the same type using SI and some non-SI units.

Science uses a specific system of units to describe measurements that are made. In chemistry, measurements are made using the **International System (SI)** of units. Most countries around the world use and understand these units as they are internationally accepted in science, commerce, sport and everyday life.

MEASUREMENT AND UNITS

Scientists use conventional ways of writing numerical measurements, such as SI units. Make sure the units you measure or observe are accurate and remember to use SI units when recording your evidence. Table 1.4.1 presents common quantities and SI units used in chemistry.

TABLE 1.4.1 Common quantities and SI units used in chemistry

Quantity	Symbol for quantity	Unit
mass	m	gram (g) kilogram (kg)
volume	V	litre (L) millilitre (mL)
amount of substance	n	mole (mol)
molar mass	M	grams per mole ($g\,mol^{-1}$)
relative molecular or formula mass	M_r	no units; relative to one atom of ^{12}C exactly
relative atomic mass	A_r	no units; relative to one atom of ^{12}C exactly
energy	E	joule (J) kilojoule (kJ)
concentration (molarity)	c	moles per litre ($mol\,L^{-1}$, M or $mol\,dm^{-3}$)
density	d	$g\,mL^{-1}$ or $kg\,L^{-1}$
temperature	T	°C, K
pressure	P	Pa

Correct use of unit symbols

The correct use of unit symbols removes ambiguity, as symbols are recognised internationally. Some important points to keep in mind when writing units and recording measurements and numbers are given in Table 1.4.2.

Upper case letters are only used for the *symbols* of the units that are named after people. For example, the unit of energy is joule and the *symbol* is J. The joule was named after James Joule who was famous for studies into energy conversions. The exception to this rule is 'L' for litre. Upper case 'L' is used because a lower case 'l' looks like the numeral '1'.

The product of a number of units is shown by separating the symbol for each unit with a space. The division or ratio of two or more units can be shown in fraction form, using a slash, or using negative exponents. Prefixes should not be separated by a space.

TABLE 1.4.2 Examples of correct and incorrect use of symbols for derived units

Rule	✓	✗
Numbers and symbols should not be mixed with words.	Thirty grams 30 g	thirty g 30 grams
Do not put spaces between prefixes and unit symbols.	kg mL kPa	k g m L k Pa
Write the correct case for symbols (upper or lower case).	1 mm 84 kg 5.2 mL	1 Mm 84 KG 5.2 ml
SI units should not be followed by a full stop unless they are at the end of a sentence. The symbols for units are not abbreviations.	12.1 mm	12.1 mm.
Only use upper case letters for unit symbols named after people. The exception is 'L' for litre, to avoid confusion because 'l' looks like the numeral '1'.	J (the unit of energy is joule, named after James Joule)	j
Units can take the plural form by adding an 's' when used with numbers greater than one. Never do this with the unit symbols.	Two kilojoules 2 kJ	2 kJs
The product of two or more units is shown by separating the symbol for each unit with a space.	0.1 mol dm^{-3}	0.1 moldm^{-3}
The division or ratio of two or more units can be shown in fraction form, using a slash, or using negative exponents.	0.1 mol dm^{-3} 0.1 mol/dm^3	0.1 mol/dm^{-3}
When units are displayed with a negative exponent such as g mL^{-1}, the negative value of the exponent signifies the division of the units, or per unit. In this case, g mL^{-1} is the same as g/mL, or grams per millilitre.	1000 kJ mol^{-1} 13°C/g	1000 kJ/ mol^{-1} 13°C/g^{-1}

Table 1.4.3 provides some examples of correct and incorrect use of symbols for derived units.

TABLE 1.4.3 Examples of the use of symbols for derived units

Correct symbol ✓	Incorrect symbol ✗
J g^{-1} °C^{-1}	J g^{-1} °C^{-1}
g mol^{-1}	gmol-1
kPa	K Pa

When units are displayed with a negative exponent, such as mol L^{-1}, the negative value of the exponent signifies the division of the units; in other words, per unit. In this case, mol L^{-1} is the same as mol/L, or moles per litre.

Worked example 1.4.1

CALCULATIONS WITH UNIT CONVERSIONS

Calculate how many litres are in one cubic kilometre.	
Thinking	**Working**
Write each volume in terms of m^3. (Remember that a km^3 is a cube that has sides of 1000 m by 1000 m by 1000 m.)	1000 L = 1 m^3 so 1 L = 0.001 m^3 1 km^3 = 1000 m × 1000 m × 1000 m = 10^9 m^3
Divide the volumes.	number of litres = $\frac{10^9}{0.001} = 10^{12}$
Check that your answer makes sense.	A litre is much smaller than a cubic kilometre, so the answer should be very large.
State the answer.	There are 10^{12} or one trillion litres in one cubic kilometre.

➤ Try yourself 1.4.1

CALCULATIONS WITH UNIT CONVERSIONS

If a person weighs 6.0×10^{1} kg and the mass of a single carbon atom is 1.99×10^{-23} g, calculate how many carbon atoms would be needed to equal the mass of the person.

1.4 Review

SUMMARY

- Scientists use conventional ways of writing numerical measurements such as using International System (SI) units.
- Units with a prefix need to be converted into scientific notation before they can be used in a chemistry formula.
- When units are displayed with a negative exponent, the negative value of the exponent signifies the division of the units. For example, gmL^{-1} is the same as g/mL or grams per millilitre.
- When writing and recording measurements, remember:
  - numbers and symbols should not be mixed with words
  - do not put spaces between prefixes and unit symbols
  - use the correct case for symbols (upper or lower case).

KEY QUESTIONS

Describe

1 State the standard unit of measurement, and the symbol, for the following quantities.

a time
b temperature
c length
d mass

2 List the following prefixes from largest to smallest: centi, milli, deci, mega, kilo, nano, micro.

Apply

3 Explain why it is important that general society, not just the scientific community, needs a systematic and consistent set of units for measurement.

Analyse

4 Convert 30.00 mL into L.

5 Identify any errors in the measurements below and correct them.

a $23\,mL/gh^{-1}$
b $79\,kls^{-1}$
c four litres
d 1.56 grams

6 Determine how many metres there are in the 656 nm wavelength of red light emitted from hydrogen.

7 Determine how many atoms there are in 5.3 g of helium.

1.5 Measuring precision and accuracy using uncertainties and percentage error

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- explain the difference between accuracy and precision
- explain the difference between uncertainty and error
- calculate uncertainty and error values for measurements
- write measurements with uncertainty and error values
- write measurements and calculations to the correct number of significant figures
- perform calculations that contain uncertainty or error values
- understand that all measurements made in chemistry experiments are subject to a level of uncertainty
- differentiate between accuracy and precision, and know how to express these quantitatively using significant figures
- perform calculations using significant figures
- explain the difference between mistakes, systematic uncertainties and random uncertainties
- determine the absolute measurement uncertainty of a value based on the precision of the instrument
- determine the uncertainty of a mean using the range of trials
- convert between absolute and percentage uncertainties
- calculate a value along with the associated uncertainty.

All measurements are limited by the instrument used and the observer. Accuracy of the measurements and results are therefore affected. Instruments have a prescribed level of precision and cannot measure within the smallest increment of the device. In addition, a scientist's technique and experience with the instrument influences the precision with which the reading can be made.

However, in science it is impossible to measure the true value, as there will always be some degree of **uncertainty**. This results in **error** and uncertainty in the values measured or observed. Therefore, science can be thought of as developing evidence-based results that have some limitations. Measurements with uncertainty and errors are normal in science and so results are always presented with a **range** (e.g. ±0.5) indicating possible precision, or processed through statistical calculations.

ACCURACY AND PRECISION

In science and statistics, the terms *accuracy* and *precision* have very specific and different meanings.

- **Accuracy** is the ability to obtain the correct measurement. To obtain accurate results, you must minimise **systematic errors**.
- **Precision** is the ability to consistently obtain the same measurement. To obtain precise results, you must minimise **random errors**.

To understand more clearly the difference between accuracy and precision, think about aiming at the bullseye on a target (Figure 1.5.1). Accuracy is being able to hit the bullseye, whereas precision is being able to hit the same spot every time. In summary, measurements should be both as precise and accurate as possible.

Any measurement made in chemistry needs to be both accurate and precise.

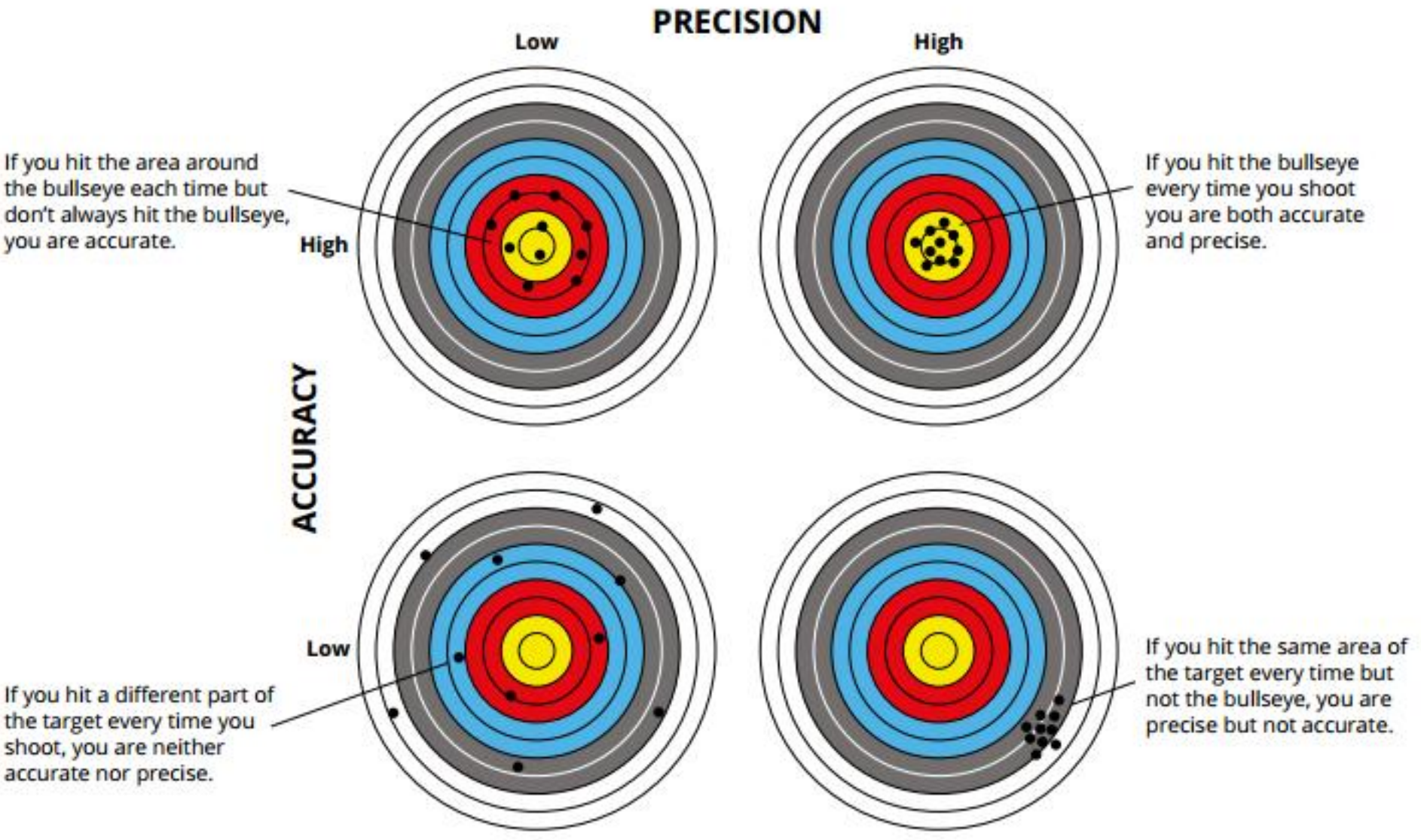

PRECISION
Low
High
If you hit the area around the bullseye each time but don't always hit the bullseye, you are accurate.
High
If you hit the bullseye every time you shoot you are both accurate and precise.
ACCURACY
Low
If you hit a different part of the target every time you shoot, you are neither accurate nor precise.
If you hit the same area of the target every time but not the bullseye, you are precise but not accurate.

FIGURE 1.5.1 An example of a target illustrates the difference between accuracy and precision.

Recording numerical data

When using instruments to measure data, the number of significant figures (or digits) and decimal places you use is determined by how precise your measurements are.

The overall precision of the measurement depends on the scale, accuracy and precision of the instrument and the technique you are using (Figure 1.5.2). For example, a beaker may be used to measure volumes approximately and has limited accuracy of, for example, ±5%; however, a graduated pipette is much more accurate, with accuracies of ±0.1% or ±0.2%. In addition, your pipette may be accurate but if your technique using the pipette is variable, the overall accuracy and precision will be limited.

When you record **raw data** and report **processed data**, you must use the number of significant figures available from your equipment or **observation**. (This is discussed in more detail in Module 1.11.) Using either a greater or smaller number of significant figures can be misleading. For example, Table 1.5.1 shows measurements of five mass samples taken using an electronic balance accurate to 2 decimal places. The data was entered into a spreadsheet to calculate the mean, which was displayed with 4 decimal places. You would record the mean as 20.83 g, not 20.8260 g, because 2 decimal places is the precision limit of the instrument. Recording 20.8260 g would be an example of false precision.

FIGURE 1.5.2 A 5 mL graduated pipette can measure volumes to an accuracy of one-tenth of a millilitre. The pipette has major divisions of 1 mL and minor divisions of 0.1 mL.

TABLE 1.5.1 An example of false precision in a data calculation

Sample	1	2	3	4	5	Mean
Mass (g)	20.13	20.62	21.22	20.99	21.17	20.8260

UNCERTAINTY AND ERROR

Uncertainty is a range of measurements from an experiment, within which the true value is expected to lie. Due to variations, an estimation is made to suggest where the true value should be found among the measurements. Expressed as a ± value, uncertainty can be derived either from the known precision of the equipment or alternatively from calculations involving the range of trials (see 'measurement uncertainty' and 'uncertainty of the mean').

Error is the difference between a measurement and the true value. This is not just an indication of human error or mistakes but is due mainly to the unlikelihood of recording the true value in any given measurement. It is due to an inability to achieve the true value. Error cannot be eliminated, and therefore it is important to understand, record and report it. Two types of error can occur—systematic error and random error (Table 1.5.2).

TABLE 1.5.2 Systemic and random errors

Error	Definition	Cause	Example
systematic	An error in measurements caused by the design of a system (e.g. methodology) or instrument (uncalibrated), which results in the measurements shifting in a systematic direction. The mean may be displaced or varied in a predictable way affecting the accuracy of the measurement. It is quantified by calculating percentage error.	• instrument calibration • choice of instrument • precision of instrument (increments) • precision of instrument (sample rate, samples per second) • sampling (the choice of population or representatives) • heat loss to the surroundings	The balance used for weighing out samples reads 0.05 g too high for all your masses because it was improperly tared (set to zero) at the start of the experiment.
			Using a standard hydrochloric acid solution for a series of titrations that is not 1.0 M. As long as the actual concentration of the acidic solution is determined, the number of moles of base required to neutralise it in each titration can be corrected for.
random	An error that affects the measurement in an unpredictable way, resulting in an even variation (fluctuation) in measurements above and below the expected true value. This affects the precision of the measurement. It is quantified by calculating uncertainty.	• estimation (measuring between increments) • sampling (frequency, spread, increments) • parallax (incorrect angle for viewing instrument scale) • instrument sensitivity • noise (random irregularity)	Using a universal indicator to determine the pH of a solution, in which the pH must be estimated by the shade and colour of the paper (e.g. yellow/orange versus bright orange).
			Measuring the time taken for a reaction to occur has a random error associated with the identification of when the reaction is judged to be complete.

Uncertainties and errors should always be calculated or measured and then reported. They then form part of the analysis and interpretation (see Module 1.7 Data analysis).

Calculating uncertainty in measurement

The goal when taking measurements is to obtain repeat values (trials) that closely agree. We expect repeat measurements to vary somewhat based on the precision of the equipment. For example, when using a measuring cylinder for the volume of solution, the **measurement uncertainty** of an analog instrument is half the smallest increment (for digital it is the smallest decimal place on the readout). Using the particular instrument, the true value is expected to fall within this range (e.g. measured value ± 0.15 mL, for a 150 mL volumetric cylinder).

$$\text{measurement uncertainty} = \pm \frac{\text{smallest increment}}{2}$$

When averaging repeat measurements, the uncertainty should be reported alongside your average. Known as **uncertainty of the mean** it represents the precision of the method expressed as the range of experimentally obtained values. The following equation is a simple way to calculate the uncertainty of the mean.

$$\text{uncertainty of the mean} = \pm \frac{\text{upper value} - \text{lowest value}}{2}$$

Worked example 1.5.1

CALCULATING UNCERTAINTY OF THE MEAN

A titration was performed three times and the volume of acid required to neutralise the solution was 20.8, 21.4 and 20.2 mL. The average volume of acid used was 20.8 mL. Calculate the uncertainty of the mean, then write the average volume including the uncertainty.

Thinking	Working
Write the formula.	$\text{uncertainty} = \pm\frac{\text{upper value} - \text{lowest value}}{2}$
Insert the values and then calculate.	$\text{uncertainty} = \pm\frac{(21.4 - 20.2)}{2}$ $= \pm\frac{1.2}{2}$ $= 0.6\,\text{mL}$
Combine measurement with uncertainty.	$20.8\,\text{mL} \pm 0.6\,\text{mL}$

➤ Try yourself 1.5.1

CALCULATING UNCERTAINTY OF THE MEAN

The rate of the reaction between sodium thiosulfate and sulfuric acid was measured by timing how long it took for the reaction mixture to turn opaque. The reaction was performed three times at each concentration of sulfuric acid and the average was calculated. For the 1.0 M solution, the time taken was 51, 47 and 58 s. The average time was 52 s. Calculate the uncertainty of the mean, then write the average time including the uncertainty.

In experimental investigations where a number of trials are performed, you have the opportunity to describe the level of uncertainty in two numerical ways, measurement uncertainty and uncertainty of the mean. When these uncertainties are expressed in the same units as the value they describe, they are an **absolute uncertainty** (e.g. 50 cm ± 0.5 cm).

SKILLBUILDER 1.5.1

Calculating absolute measurement uncertainty

Calculate the absolute measurement uncertainty for instrumental error during an experiment where the temperature was measured at 32°C using a glass thermometer with increments of 1°C and also a digital thermometer with increments of 0.1°C.

For the glass thermometer

1 Write down the formula.

$$\text{uncertainty} = \pm\frac{\text{smallest increment}}{2}$$

2 Insert the values and calculate.

$$\text{uncertainty} = \pm\frac{1}{2}$$
$$= \pm 0.5°\text{C}$$

3 Combine the measurement with the uncertainty.

$32°\text{C} \pm 0.5°\text{C}$

For the digital thermometer

1 Write down the formula.

$\text{uncertainty} = \pm$ smallest increment

2 Insert the values and calculate.

$\text{uncertainty} = \pm 0.1$

3 Combine the measurement with the uncertainty.

$32.0°\text{C} \pm 0.1°\text{C}$

Uncertainty can also be reported as a percentage of the measurement; this is known as **percentage uncertainty**. To calculate the percentage uncertainty, apply this formula:

$$\text{percentage uncertainty} = \pm\left(\frac{\text{absolute uncertainty}}{\text{measurement}}\right) \times 100$$

Worked example 1.5.2

CALCULATING PERCENTAGE UNCERTAINTY FOR INSTRUMENTAL ERROR

The temperature during an experiment was measured and then reported at 32.00°C ± 0.05°C. Calculate the percentage measurement uncertainty. Write the temperature with the uncertainty.

Thinking	Working
Write the formula for percentage uncertainty.	percentage certainty $= \pm\left(\frac{\text{absolute uncertainty}}{\text{measurement}}\right) \times 100$
Insert the values and calculate.	percentage uncertainty $= \pm\left(\frac{0.05}{32}\right) \times 100$ $= 0.16\ \%$
Combine the measurement with the percentage uncertainty and express to the appropriate number of significant figures.	32.00°C ± 0.16%

➤ Try yourself 1.5.2

CALCULATING PERCENTAGE UNCERTAINTY FOR INSTRUMENTAL ERROR

The pH of a solution was determined to be 11.4 ± 0.6. Calculate the percentage measurement uncertainty. Write the pH with the uncertainty.

Calculating percentage error in values

As stated above, scientists try to calculate the 'true' or 'correct' value. However, due to equipment and/or method, experimental results may give an inaccurate value. The percentage error between the measured value and the true value provides information about validity and systematic error (see Part B) and can be calculated using the percentage error formula:

$$\text{percentage error (\%)} = \left|\frac{\text{measured value} - \text{true value}}{\text{true value}}\right| \times \frac{100}{1}$$

This formula can also be used to calculate the difference between the true value and the generally accepted value of a quantity such as the density of water. The density of water is generally stated to be $1\,\text{kg}\,\text{m}^{-3}$; however, the exact density at 4.0°C is $0.999\,839\,5\,\text{kg}\,\text{m}^{-3}$. This calculation is shown in Worked example 1.5.3.

In this case the measured value is replaced with the accepted value. The percentage error in the accepted (rounded) value of $1\,\text{kg}\,\text{m}^{-3}$ is less than 0.02%. This indicates that using $1\,\text{kg}\,\text{m}^{-3}$ is acceptable since the percentage error is very small and likely to be much smaller than experimental uncertainty.

Worked example 1.5.3

CALCULATING PERCENTAGE ERROR

Calculate the percentage error between the true density of water at 4.0°C ($0.9998395\,kg\,m^{-3}$) and the generally accepted (rounded) value of $1\,kg\,m^{-3}$.

Thinking	Working
Write the formula.	$\text{percentage error}(\%) = \left\lvert \frac{\text{measured value} - \text{true value}}{\text{true value}} \right\rvert \times \frac{100}{1}$
Insert the values and then calculate.	$\text{percentage error } (\%) = \left\lvert \frac{1 - 0.9998395}{0.9998395} \right\rvert \times \frac{100}{1}$ $= \frac{0.0001605}{0.9998395} \times \frac{100}{1}$ $= 0.01605\,\%$

➤ Try yourself 1.5.3

CALCULATING PERCENTAGE ERROR

The laboratory technician made up a standard solution of 0.200 M. A student calculated the concentration of the solution to be 0.185 M. Calculate the percentage error.

Significant figures

When measuring phenomena during experimentation, the precision of the instruments determines the number of significant figures and decimal places you record in the data.

Significant figures convey meaning and precision and the number of significant figures used depends on the scale of the instrument. You should record data using the number of significant figures available from the equipment or observation. Using either a greater or smaller number of significant figures is misleading.

When writing an answer to the correct number of significant figures, you may need to use rounding if the initial answer has more figures (digits) than you need. These extra figures are called 'non-significant figures'. If the first non-significant figure is ≥5, round up the number. If the first non-significant figure is <5, then do not round up. For example, if the initial answer for a calculation was 2.1259 but you only needed an answer to 3 significant figures, you would round it to 2.13. If the initial answer was 2.1241, this becomes 2.12, rounded to 3 significant figures.

SKILLBUILDER 1.5.2

Identifying significant figures

When giving an answer to a calculation, it is important to take note of the number of significant figures that you use.

You should give an answer that is as accurate as possible. However, an answer cannot be more precise than the data or the measuring device used to calculate it. For example, if an electronic balance that measures to the nearest gram shows that an object has a mass of 56 g, then the mass should be recorded as 56 g, not 56.0 g. This is because you do not know whether it is 56.0 g or 56.1 g or 56.2 g or 55.8 g.

The number 56 has 2 significant figures. Recording to 3 significant figures (e.g. 56.0 g or 55.8 g) would not be scientifically 'honest'.

If this mass of 56 g is used to calculate another value, it would also not be 'honest' to give an answer that has more than 2 significant figures.

Determining the number of significant figures to give in an answer depends on the kind of calculation you are doing.

- If you are multiplying or dividing, use the smallest number of significant figures provided in the initial values.
- If you are adding or subtracting, use the smallest number of decimal places provided in the initial values.

Working out the number of significant figures

Use the following rules to avoid confusion in determining how many significant figures are in a number.

1. All non-zero digits are always significant; for example, 21.7 has 3 significant figures.
2. All zeros between two non-zero digits are significant; for example, 3015 has 4 significant figures.
3. A zero to the right of a decimal point and following a non-zero digit is significant; for example, 0.5700 has 4 significant figures.
4. Any other zero is not significant, as it will be used only for locating decimal places; for example, 0.005 has just 1 significant figure.

Worked example 1.5.4

IDENTIFYING SIGNIFICANT FIGURES

a Identify which of the following is written to 2 significant figures.

A 30.1
B 0.00040
C 0.5
D 5.12

b George multiplied 1.22 by 1.364. Identify which of the options below shows the result of this multiplication with the correct number of significant figures.

A 1.66
B 1.664
C 1.65
D 1.7

Thinking	Working
a The zeros that come before the non-zero digit 4 are not significant, whereas those that follow 4 are significant.	B is correct. A has 3 significant figures. C has 1 significant figure. D has 3 significant figures.
b 1.22×1.364 $= 1.66408$	A is correct. When two numbers are multiplied, use the smallest number of significant figures in the initial values to report your answer. In George's multiplication, the answer is 1.66408, but since 1.22 has only 3 significant figures, the correct answer is 1.66.

➤ Try yourself 1.5.4

IDENTIFYING SIGNIFICANT FIGURES

Identify which of the following is written to 4 significant figures.

A 0.0041
B 0.410
C 41.00
D 4100

Worked example 1.5.5

ACCURATELY RECORDING MEASUREMENTS FROM INSTRUMENTS

When measuring the amount of solution for an acid-base experiment, you need to record the results accurately and be able to identify the appropriate number of significant figures to use. The numbered markings on the pipettes below are in mL.

a State the measurement for the liquid level shown on this plastic pipette and identify the number of significant figures in this result.

b State the measurement for the liquid level shown on this glass pipette and identify the number of significant figures in this result.

Thinking	Working
a The increments shown on the plastic pipette determine the accuracy with which the measurement can be recorded. If you add extra numbers or remove numbers it becomes inaccurate.	The plastic pipette is marked with increments of 0.05 mL; therefore all results must be recorded to the nearest 0.05 mL, with 2 decimal places.
Determine where the meniscus (the lowest point) of the liquid falls.	The meniscus of the liquid in the pipette is closest to the 2.00 mL marking, therefore the result must be recorded as 2.00 mL, not as 2.0 mL
Determine the number of significant figures included in this result.	The measurement of 2.00 mL has 3 significant figures.
b The increments shown on the glass pipette determine the accuracy with which the measurement can be recorded. If you add extra numbers or remove numbers, it becomes inaccurate.	The glass pipette is marked with increments of 0.05 mL, therefore all results must be recorded to the nearest 0.05 mL, with 2 decimal places.
Determine where the meniscus (the lowest point) of the liquid falls.	The meniscus of the liquid in the pipette is closest to the 2.00 mL marking, therefore the result must be recorded as 2.00 mL, not as 2 mL.
Determine the number of significant figures included in this result.	The measurement of 2.00 mL has 3 significant figures.

➤ Try yourself 1.5.5

ACCURATELY RECORDING MEASUREMENTS FROM INSTRUMENTS

When measuring the temperature for a calorimeter experiment, you need to record the results accurately and be able to identify the appropriate number of significant figures to use.

a State the measurement shown on this glass alcohol thermometer, and identify the number of significant figures in this result.

b State the measurement shown on this digital thermometer, and identify the number of significant figures in this result.

Significant figures are the exact digits observed when recording the results of an observation or experiment. For example, if the volume of O_2 gas produced and measured from the electrolysis of water in a 20-minute experiment was 6.0 mL because exactly 6.0 mL was observed, then the measurement is 6.0 mL with 2 significant figures, not 6 mL.

Table 1.5.3 shows some examples of measurements and how many significant figures they have.

TABLE 1.5.3 Measurements and significant figures

Measurement	Number of significant figures
15	2
3.5	2
3.50	3
0.037	2
1401	4
1400	2

Using either a greater or smaller number of significant figures can be misleading. For example, Table 1.5.4 shows three measurements to 2 decimal places (4 significant figures). The data was entered into a spreadsheet to calculate the mean, which was displayed with 3 decimal places. You would record the mean as 19.52 mL, not 19.517 mL, because 2 decimal places is the precision limit of the instrument. Recording 19.517 g would be an example of false precision.

TABLE 1.5.4 An example of false precision in a data calculation

Trial	1	2	3	Mean
Volume (mL)	19.45	19.55	19.55	19.517

It is important to record the exact numbers measured during an experiment. This determines the significant figures, and later the accuracy and precision of the analysis. If a zero is observed, record it, as it is the exact amount measured. This includes all zeros before and after decimal places.

Determining uncertainty in a single measurement

When using an instrument to measure a property of an object, there will always be a limit as to how precise the reading can be.

The precision that can be read off a single instrument is called the limit of reading. This is the smallest visible increment on an analog instrument, or if a digital instrument is used, then the limit of reading is usually the smallest decimal place given on the screen.

For most analog instruments, the absolute uncertainty, Δx, in a measurement of x is exactly half of the limit of reading for each part of the measured object that has to be lined up. This means that the actual measurement could be anywhere from *half* of the smallest increment too big to *half* of the smallest increment too small.

Some analog instruments have a zero mark and a reading mark, such as a ruler shown in Figure 1.5.3a. The object to be measured has to be lined up at *both* ends, thus doubling the absolute uncertainty. For instance, when using rulers or burettes, the absolute uncertainty is equal to the limit of reading, rather than half of it.

In a digital instrument, Δx is typically the limit of reading, or the smallest decimal place given on the screen. An example of this is a high-precision electronic balance as shown in Figure 1.5.3b.

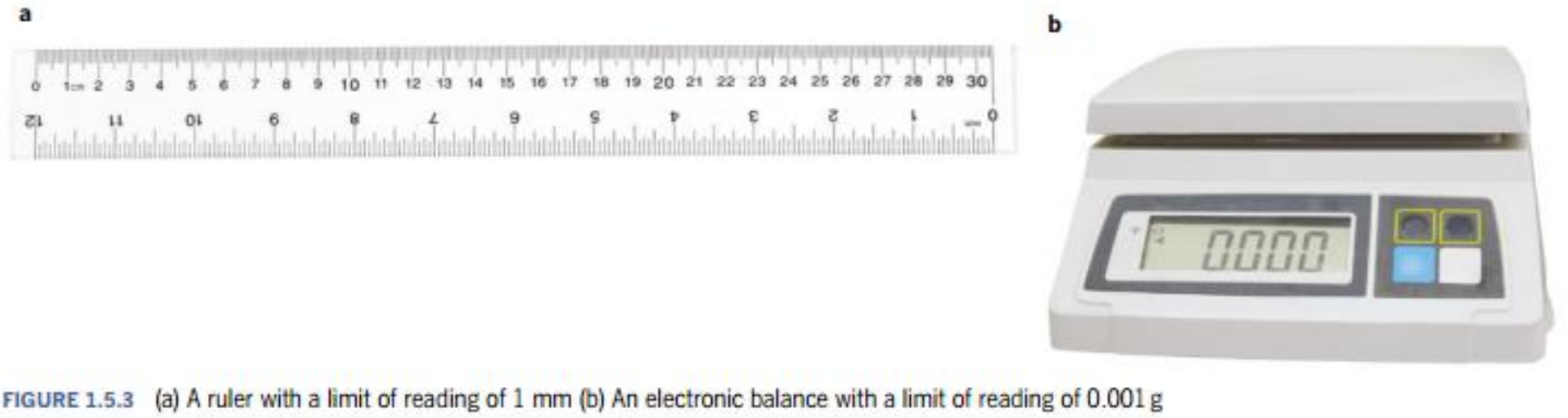


FIGURE 1.5.3 (a) A ruler with a limit of reading of 1 mm (b) An electronic balance with a limit of reading of 0.001 g

Usually, the absolute measurement uncertainty in a measurement will have one significant figure, or two significant figures if the first digit is 1. This is done because the uncertainty of a measurement is meant to be an estimate and writing more than two significant figures is therefore unhelpful.

> For analog instruments that have one scale to line up (such as a measuring cylinder, thermometer or voltmeter), the absolute measurement uncertainty is half of the smallest increment scale, or limit of reading.
>
> For analog instruments that have two scales to line up (such as rulers and burettes), the absolute measurement uncertainty is equal to the smallest increment scale, or limit of reading.
>
> For digital instruments, the absolute measurement uncertainty is equal to the smallest decimal place displayed.

When the absolute uncertainty has been determined, the measurement should be rounded so that it and the absolute uncertainty have the same number of *decimal places*. This is to keep the measurement and its uncertainty to the same precision. Examples of measurements and their absolute uncertainties are shown in Table 1.5.5.

TABLE 1.5.5 Examples of writing a measurement and its absolute uncertainty

Measurement and absolute uncertainty	Comments
48.2 ± 1.0°C	The absolute uncertainty is written to 2 significant figures because the first digit is 1. The measurement and uncertainty then have the same number of decimal places.
99.99 ± 0.01 s	The measurement and absolute uncertainty are written to 2 decimal places, with one significant figure for the uncertainty. This measurement of time may have been recorded using a digital device, such as a data logger, since the precision is quite high.
0.000000031 ± 0.000000005 kg	This is technically a correct way of writing a measurement and its absolute uncertainty, but it is normally written in scientific notation so that the measurement and uncertainty have the same power of ten, i.e. $(3.1 \pm 0.5) \times 10^{-8}$ kg

The limit of reading and absolute uncertainties of common equipment used in a chemistry laboratory are shown in Table 1.5.6.

TABLE 1.5.6 A summary of common instruments and their uncertainties

Instrument	Type of instrument	Limit of reading	Absolute uncertainty	Example	Notes
mm ruler	analog	1 mm	± 1.0 mm	123.8 ± 1.0 mm	Half of the limit of reading is 0.50 mm, but since the object to be measured has to be lined up at both ends, the uncertainty is double this, or ±1.0 mm.
cm ruler	analog	1 cm	± 1.0 cm	31.4 ± 1.0 cm	Half of the limit of reading is 0.50 cm, but since the object to be measured has to be lined up at both ends, the uncertainty is double this, or ±1.0 cm.
thermometer	analog	1.0°C	± 0.5°C	24.4 ± 0.5°C	Only the top part of the liquid in the thermometer has an uncertainty, so the uncertainty is exactly half of the limit of reading.
measuring cylinder	analog	1.0 mL	± 0.5 mL	15.7 ± 0.5 mL	The limit of reading and absolute uncertainty depend on the size of the measuring cylinder.
burette	analog	0.1 mL	± 0.1 mL	20.10 ± 0.1 mL	Half of the limit of reading is 0.05 mL, but since the object to be measured has to be lined up at both ends, the uncertainty is double this, or ±0.1 mL.
volumetric pipette	analog	varies	varies ± 0.03 mL	25.00 ± 0.03 mL	The uncertainty for the pipette is based on the precision given on the pipette. The precision varies based on the size and quality of the pipette.
stopwatch	digital	0.01 s	from ± 0.1 to ± 0.4 s	9.6 ± 0.2 s	The limit of reading is not the absolute uncertainty for a stopwatch because the user's reaction time (usually between 0.1 and 0.4 s) needs to be taken into consideration.
electronic balance	digital	typically 0.01 g	± 0.01 g	7.03 ± 0.01 g	The limit of reading is usually the smallest decimal place given on the screen.

The absolute uncertainty should be written to 1 or a maximum of 2 significant figures.

These steps will help you write a measurement and its absolute uncertainty.

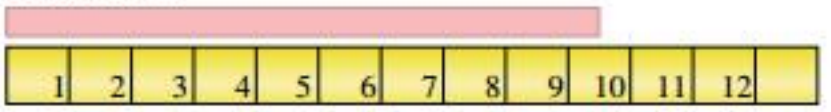
1. Determine the absolute uncertainty from the type of instrument used to measure the quantity.
2. Measure the quantity, including an estimate of the final significant figure.
3. If the first digit of the absolute uncertainty is 1, then one more significant figure can be quoted. Usually this extra digit is zero.
4. The measurement is then rounded up or down to the same number of decimal places, or place value holders, as the uncertainty; however, the uncertainty should not be presented to more than 2 significant figures.
5. Do not forget the unit of measurement for the quantity.

Worked example 1.5.6

READING MEASUREMENTS

For each of the following objects, determine its measurement and uncertainty.

a the length of the pink rectangle measured with a ruler calibrated in centimetres



b the temperature of tap water measured using an analog thermometer

c the temperature of tap water measured using a digital thermometer

Thinking	Working
a The pink rectangle is between 9 cm and 10 cm in length, so the best estimate for this is 9.5 cm.	length, $L = 9.5\,\text{cm}$
The limit of reading is 1.0 cm, so this is the uncertainty in a centimetre ruler.	$\Delta L = \pm 1.0\,\text{cm}$
Write the measurement and uncertainty.	length = 9.5 ± 1.0 cm

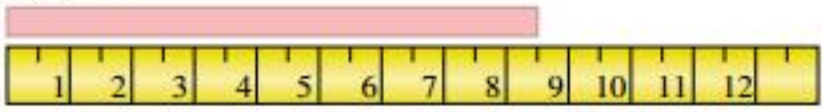
b The temperature is between 20°C and 21°C, with the best estimate of 20.2°C.	temperature, $T = 20.2°C$
The limit of reading is 1.0°C, so the uncertainty is half of this, i.e. 0.5°C.	$\Delta T = \pm 0.5°C$
Write the measurement and uncertainty.	temperature = 20.2 ± 0.5°C
c This temperature measurement is done using a digital thermometer, so the temperature is simply read off the screen at 31.2°C.	temperature, $T = 31.2°C$
The uncertainty in this measurement is equal to the smallest decimal value displayed, i.e. ± 0.1°C.	$\Delta T = \pm 0.1°C$
Write the measurement and uncertainty.	temperature = 31.2 ± 0.1°C

➤ Try yourself 1.5.6

READING MEASUREMENTS

For each of the following objects, determine its measurement and uncertainty.

a the length of the pink rectangle measured with a ruler with increments of 0.5 cm.



b a red liquid in an analog measuring cylinder

c the mass of this donut measured on an electronic balance

Worked example 1.5.7

CALCULATING THE TOTAL UNCERTAINTY

Determine the uncertainty in the number of moles of NaOH in a 25 mL 1.00 ± 0.05 M NaOH solution measured out using a 25.00 ± 0.05 mL pipette.

Thinking	Working
Write the formula.	number of moles = volume × concentration
How to propagate the uncertainty:	Since the number of moles is calculated by multiplying the volume by the concentration, the total uncertainty is determined by the sum (addition) of the percentage uncertainties for each quantity.
Calculate the percentage uncertainties for each measurement.	percentage uncertainty of concentration $= \frac{\text{absolute uncertainty}}{\text{measurement}} \times \frac{100}{1}$ $= \frac{0.05}{1.00} \times \frac{100}{1}$ $= 5\%$ percentage uncertainty of volume $= \frac{\text{absolute uncertainty}}{\text{measurement}} \times \frac{100}{1}$ $= \frac{0.05}{25.00} \times \frac{100}{1}$ $= 0.2\%$
Calculate the number of moles (including sum of percentage uncertainties).	number of moles = volume × concentration = 25.00 × 1.00 = 25.00 mL ± 5.2%

➤ Try yourself 1.5.7

CALCULATING THE TOTAL UNCERTAINTY

Calculate the density (including uncertainty) of a 10 ± 0.1 cm^3 block of wood weighing 24.3 ± 0.1 g.

Calculations with uncertainties

There are a few rules when conducting calculations with numbers (or measurements) that have uncertainties. It is important to record the correct uncertainty once all the calculations are done so that the appropriate accuracy is reported. Table 1.5.7 outlines the rules for undertaking calculations with data and its associated uncertainty.

Keep in mind that the rules for significant figures apply to all numerical reporting, including the uncertainties.

TABLE 1.5.7 Rules for calculations involving uncertainty

Calculation	Rule	Examples
addition and subtraction	add the absolute uncertainties	5.4 ± 0.05 + 3.2 ± 0.05 = 8.6 ± 0.1 5.4 ± 0.05 + 3.2 ± 0.1 = 8.6 ± 0.15 5.4 ± 0.05 – 3.2 ± 0.05 = 2.2 ± 0.1 5.4 ± 0.05 – 3.2 ± 0.1 = 2.2 ± 0.15
multiplication and division	add the percentage uncertainties	3.0 ± 0.05 × 1.5 ± 0.05 = 3.0 ± 1.7% × 1.5 ± 3.3% = 4.5 ± 5.0% 3.0 ± 0.05 ÷ 1.5 ± 0.05 = 3.0 ± 1.7% ÷ 1.5 ± 3.3% = 2.0 ± 5.0%
multiplying by a constant (absolute uncertainty)	multiply the uncertainty	3.14 × (4.1 ± 0.05) = 12.9 ± 0.16
multiplying by a constant (percentage uncertainty)	maintain the uncertainty	3.14 × (4.1 ± 1.6%) = 12.9 ± 1.6%

Worked example 1.5.8

PROPAGATING UNCERTAINTIES

A student uses a 20 mL pipette twice to measure out 40 mL of solution. If the uncertainty in the pipette is 0.05 mL, determine the uncertainty in the total volume measured.

Thinking	Working
How to propagate the uncertainty:	Since the total volume is determined by the sum (addition) of the volumes, the uncertainties are also summed.
Write the formula.	Add the uncertainties: total uncertainty = $\sum$uncertainty in each measurement = 0.05 + 0.05 = 0.10
Write the volume and total uncertainty.	total volume = 40.00 mL ± 0.10 mL

➤ Try yourself 1.5.8

PROPAGATING UNCERTAINTIES

A student uses a 20 mL pipette four times to measure out 80 mL of solution. If the uncertainty in the pipette is 0.05 mL, determine the uncertainty in the total volume measured.

1.5 Review

SUMMARY

- Accuracy is the ability to obtain the correct measurement. To obtain accurate results, you must minimise systematic errors.
- Precision is the ability to consistently obtain the same measurement. To obtain precise results, you must minimise random errors.
- Uncertainty is a range of measurements from the experiment in which the true value is thought to lie. It is obtained using the precision of the measuring instrument (measurement uncertainty) or by calculations of repeat trials (uncertainty of the mean).
- Error is the difference between a measurement and the true value
- Uncertainty values are presented as a range (e.g. ±0.3).
- A simple way to calculate the uncertainty of the mean is:

$$uncertainty\ of\ the\ mean = \pm\frac{(upper\ value - lowest\ value)}{2}$$

- A simple way to calculate the measurement uncertainty is:

$$measurement\ uncertainty = \pm\frac{smallest\ increment}{2}$$

- The percentage uncertainty can be calculated using this formula:

$$percentage\ uncertainty = \pm\left(\frac{absolute\ uncertainty}{measurement}\right)\times 100$$

- The percentage error, when the experimental result can be compared with a theoretical or accepted result (value), can be calculated using this formula:

$$percentage\ error(\%) = \left|\frac{measured\ value - true\ value}{true\ value}\right| \times \frac{100}{1}$$

- The rules for calculations involving uncertainty are listed in the following table.

Calculation	Rule
addition and subtraction	add the uncertainties
multiplication and division	add the percentage uncertainties
multiplying with a constant (absolute uncertainty)	multiply the uncertainty
multiplying with a constant (percentage uncertainty)	maintain the uncertainty

- Significant figures are a way of communicating how precise a measurement is.
- The number of significant figures used depends on the scale of the instrument.
- There are specific rules governing how many significant figures there can be in any measurement.
  - All non-zero digits are significant.
  - All zeros between non-zero digits are significant.
  - Trailing zeros (either decimal or not) if measured are significant.
  - Leading zeros are not significant (in numbers with decimals, they only inform where the decimal is placed).
- All measurements made in chemistry experiments are subject to a level of uncertainty or doubt as to the precision of that measurement.
- Accuracy is a description of how close a measurement is to the true value.
- Precision is a description of how many digits can be written down for a single measurement, or how close together a group of measurements are.
- Systematic errors arise due to mistakes in calibrating or using equipment the wrong way for every measurement.
- Random errors are naturally occurring and cannot be eliminated.
- The limit of reading of an instrument is the smallest increment on the instrument.
- Uncertainties are typically written as an absolute value or percentage.
- Measurement uncertainty represents the uncertainty in the readings due to limitations in equipment, reflecting the precision of the measurement. For example, if the best estimate of a volume is 5.0 cm^3 with a smallest increment of 0.2 cm^3, the measurement uncertainty is ±0.1 cm^3.
- Percentage error indicates the accuracy of the measured value by comparing the difference between the measured value and the true value. A lower percentage error signifies a more accurate measurement.
- Propagation of uncertainties involves the mathematical combination of uncertainties from a range of variables.
- When adding or subtracting measurements, the individual absolute uncertainties always add.
- When multiplying or dividing measurements, the individual percentage uncertainties always add.
- When raising a measurement to a power, the percentage uncertainty is multiplied by the absolute value of the power.
- When using measurements in a formula, perform any addition and subtraction propagations first, followed by multiplication, division and exponents.

KEY QUESTIONS

Describe

1 Describe how values of uncertainty and error are presented.

2 State the absolute uncertainty of the following instruments.

- **a** a ruler with 1 cm increments
- **b** a protractor graduated in 1° intervals
- **c** an electronic balance giving a reading to the nearest 0.001 g
- **d** an analog needle voltmeter graduated in 10 V intervals

Apply

3 Explain the difference between accuracy and precision.

4 Explain why it would be unreasonable to state that the absolute uncertainty in a handheld digital stopwatch is ± the limit of reading or ±0.01 s.

Analyse

5 Calculate the average and the uncertainty of the mean for the two sets of data below.
Data set A: 11.4, 10.9, 11.8, 10.6, 11.5, 11.1
Data set B: 25.3, 27.4, 22.0, 26.1, 28.4, 23.1

6 Determine the absolute measurement uncertainty of the following instruments.

- **a** a garden pH meter graduated in 0.2 intervals
- **b** a burette graduated in 0.1 mL intervals
- **c** an electronic balance giving a reading to the nearest 0.001 g

1.6 Tables and graphing

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- create tables to record and organise data
- present data from tables into graphs
- distinguish between types of graphs
- select appropriate graphs to represent data
- represent missing data in graphs
- explain what outliers are and know how to represent them in graphs.

PRESENTING DATA IN TABLES

Tables record number values and allow you to organise your data. In general, tables provide more detailed data than graphs, but it is easier to observe trends and patterns in data when they are in graph form than in table form.

Presenting raw data in tables

Tables organise data into rows and columns, and can vary in complexity according to the nature of your data. Tables can be used to organise raw data and processed data, or to summarise results.

The simplest form of a table is a two-column chart. The first column should contain the independent variable (the one you control) and the second column should contain the dependent variable (the one that may change in response to a change in the independent variable).

As you can see in Figure 1.6.1, tables should have the following features:

- a descriptive title
- column headings (including the units)
- aligned figures (align the decimal points)
- the independent variable placed in the left column.

Table 1. Neutralisation of excess acid from the reaction of HCl with 1.2g of calcium carbonate

concentration of HCl (M)	volume of 0.5 M NaOH ± 0.5 (mL)			
	trial 1	trial 2	trial 3	average
0.1				
0.3				
0.5				
0.7				
1.0				
2.0				

- accurate descriptive title
- dependent variable identifies the data set and shows the unit of measurement and the measurement uncertainty of the equipment
- independent variable in the left-hand column shows the units of measurement
- rows show the different concentrations of the solution used—the range of values for the independent variable
- a minimum of five different data points for the independent variable
- space for trials—in this case three repeat trials were conducted
- column to calculate the averages

FIGURE 1.6.1 Features of a good table.

Presenting processed data in tables

Table 1.6.1 shows the relationship between temperature and average reaction rate. It displays reaction rate data in a processed format, because it displays the mean of several values for each temperature. To report processed data accurately, the uncertainty is also displayed; this will be a requirement for assessments.

TABLE 1.6.1 Effect of temperature on mean reaction rate, including uncertainty

Temperature (°C)	Average reaction rate (mol dm^{-3} s^{-1})
15	0.038 ± 0.002
25	0.043 ± 0.001
35	0.059 ± 0.001
45	0.074 ± 0.002

PRESENTING DATA IN GRAPHS

A **graph** is an incredibly useful tool. In chemistry, data is plotted using a line or curved graph, which is sometimes called a scatterplot.

Plotting data in graphs has many advantages.

- Data can be represented visually.
- Data points that are incorrect can be ignored.
- Constants can be determined from the properties of the line or curve.
- Uncertainties can be represented as **error bars**.
- A general **line of best fit** that matches the trend of the majority of the data points can be determined.
- Any known relationship between the dependent and independent variables can be supported or rejected, especially by the use of uncertainties.

Tables often provide more detailed data than graphs, but graphs can suggest a possible relationship between the dependent and independent variables, and highlight if no relationship exists. From the shape of the line or curve, it is easier to observe trends, patterns and gaps in data in graph form than in table form.

Graphs, like that shown in Figure 1.6.2, are used when two variables are being considered and one variable is dependent on the other. The graph shows the relationship between the variables.

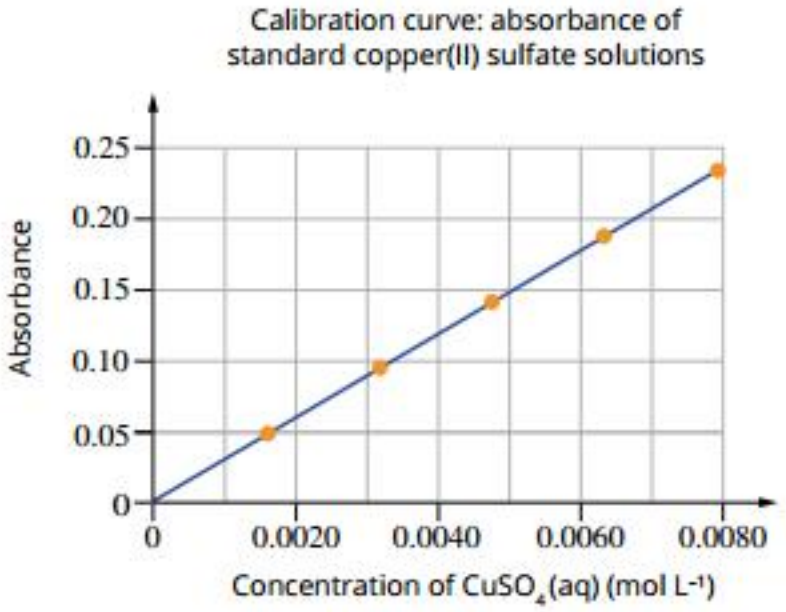


FIGURE 1.6.2 A graph showing the relationship between two variables: absorbance (dependent variable) and concentration of $CuSO_4(aq)$ (independent variable).

DRAWING GRAPHS IN CHEMISTRY

For use in chemistry, every graph must have the following features.

1 The graph must have a suitable set of axes for the independent and dependent variables.

Most chemistry graphs are only drawn in the first quadrant, but some graphs use all four quadrants (i.e. have negative values for the independent and dependent variables).

Remember that:

- the independent variable is the variable that you deliberately change and always goes on the *x*-axis
- the dependent variable is the variable that changes in response to the independent variable and always goes on the *y*-axis.

2 The graph must have a suitable scale that allows information to be seen easily and quickly.

For most graphs, it is important to choose a scale that is linear and has tick marks at common intervals (e.g. 2, 5, 10, 100 units).

3 The title and axes must have labels. Make sure that the axis labels show information about the quantity and units. Give a descriptive title that is not just a repeat of the labels of the axes.

4 Data points should be plotted as a small circle or small cross indicating their position.

5 Error bars should be drawn for each point. These indicate the absolute uncertainties in the independent (a horizontal line) and dependent (a vertical line) values. They are drawn as a horizontal line centred on the data point indicating the independent variable's uncertainty left and right of the value, and as a vertical line centred on the data point indicating the dependent variable's uncertainty above and below the value. Combining the *x* and *y* error bars forms an error rectangle, within which true measurement is located (Figure 1.6.3).

The smaller the errors bars for a given point, the more precise the measurement is.

Graph showing example of an error bar

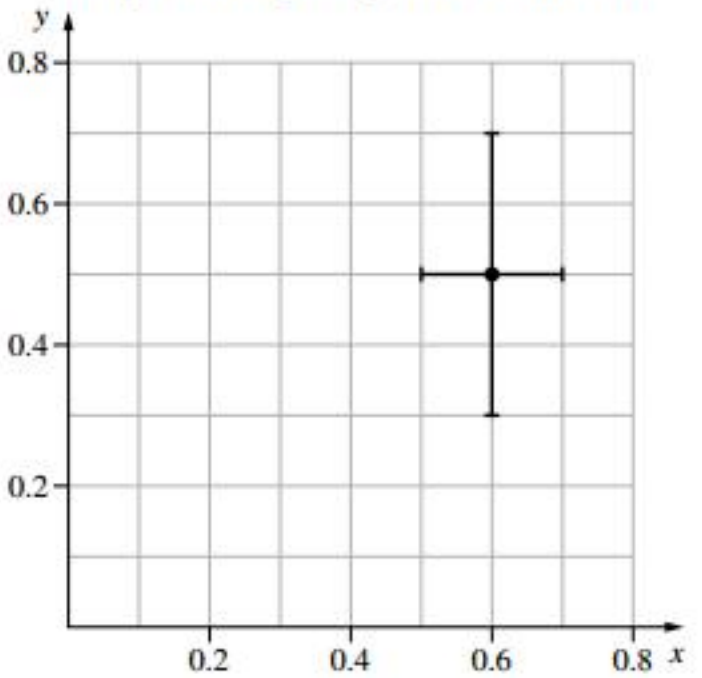


FIGURE 1.6.3 This error bar has an *x* value of 0.6 ± 0.1 and a *y* value of 0.5 ± 0.2.

Error bars are the graphical representation of the uncertainties in the independent and dependent variables.

Graph showing example of line of best fit

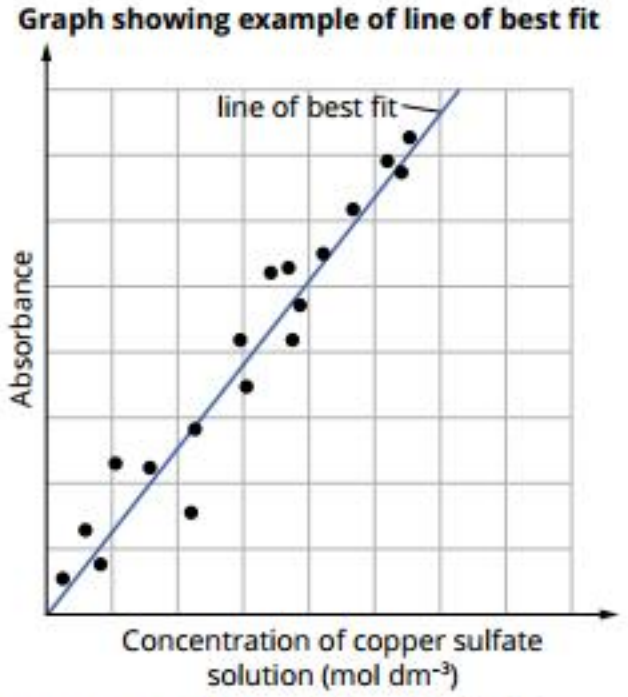


FIGURE 1.6.4 This graph shows that the line of best fit should summarise the data rather than pass through each point. It should be extrapolated so that it intersects the y-axis.

The line of best fit

This is the straight line or a curve that best summarises the data. This line does not have to pass through every point or the origin, but does have to be one smooth continuous line or curve and *not* a 'join the dots' line (Figure 1.6.4). Typically, the line of best fit should have as many points on the line as possible, but if this is not possible then it should have as many points above the line as there are below the line. The position of this line can be estimated by eye but mathematical or graphing programs can be used to determine the line of best fit more accurately.

The line of best fit is a straight line or curved line that best summarises the general pattern of the data on the graph.

These are some of the general rules to follow when making a graph.

- Keep the graph simple and uncluttered.
- Use a descriptive title.
- Represent the independent variable on the *x*-axis and the dependent variable on the *y*-axis.
- Start each axis at zero.
- Match the length of the axes to the data.
- Clearly label each axis with both the variable and the unit in which it is measured.
- Use small symbols such as circles or crosses for data points.
- Use different symbols or colours for different data sets.

TYPES OF GRAPHS SEEN IN CHEMISTRY

There are several types of graphs, including line graphs and bar graphs. The best one to use will depend on the nature of the data. In chemistry, many relationships exist between two variables and are represented as formulas and graphs. Each of the following graphs shows some particular relationship between the independent and dependent variables that occur often in chemistry.

You will encounter all of these types of graphs at some stage during your Chemistry course.

Scatterplots and line graphs

Scatterplots are commonly used to display data in the form of a graph, and can be used to plot raw or processed data. They are used to show the relationship between two variables when one variable is dependent on the other.

The independent variable, which is set by the experimenter, is always shown on the *x*-axis. The dependent variable, which is the variable measured in the experiment, is always shown on the *y*-axis. The data is plotted on the graph as a series of points. Each point should be drawn in pencil as a small circle or cross. Alternatively, you can use a computer program to generate your graphs.

A **line graph** is a good way of representing **continuous quantitative data**. In a line graph, the values are plotted as a series of points on the graph. A line can then be drawn from each point to the next, as shown in Figure 1.6.5. This line shows the change in data from one point to the next but does not predict the value of a point between the plotted data.

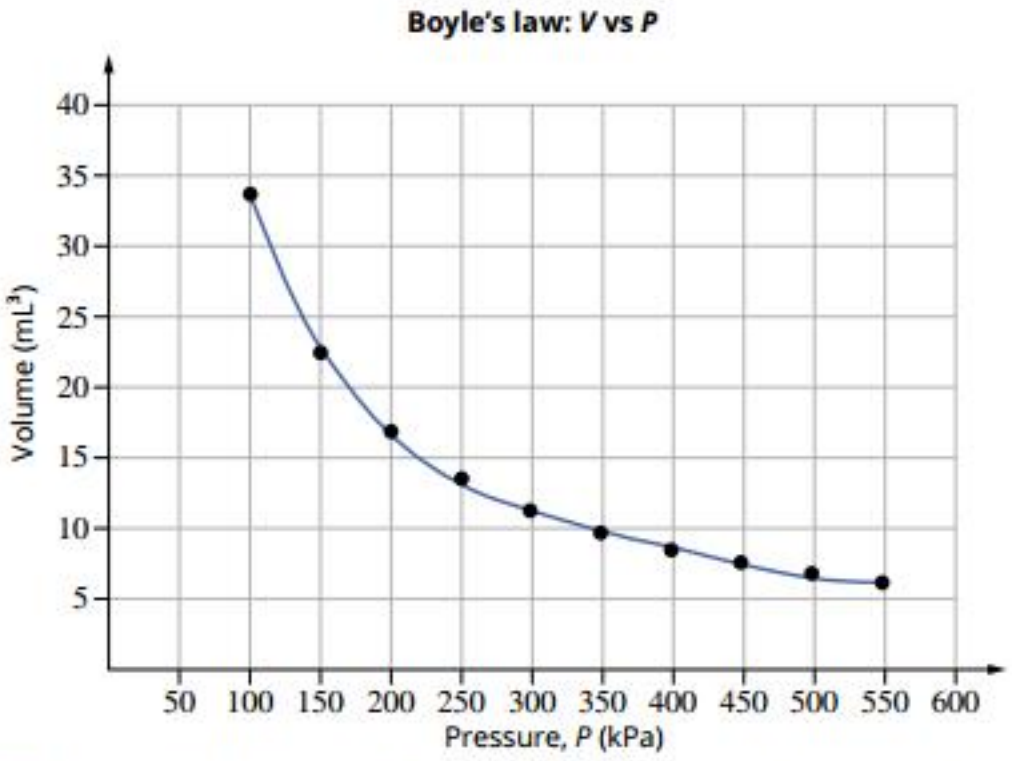


FIGURE 1.6.5 A line graph showing the change in volume of a gas in a syringe against the pressure of the gas inside.

Alternatively, a line of best fit can be drawn as a single straight or curved line, as shown in Figure 1.6.6, which is also known as a **trend line**. It is used to show the overall trend in the data, and can be used to predict values between the data points. This will be covered in more detail in Module 1.7.

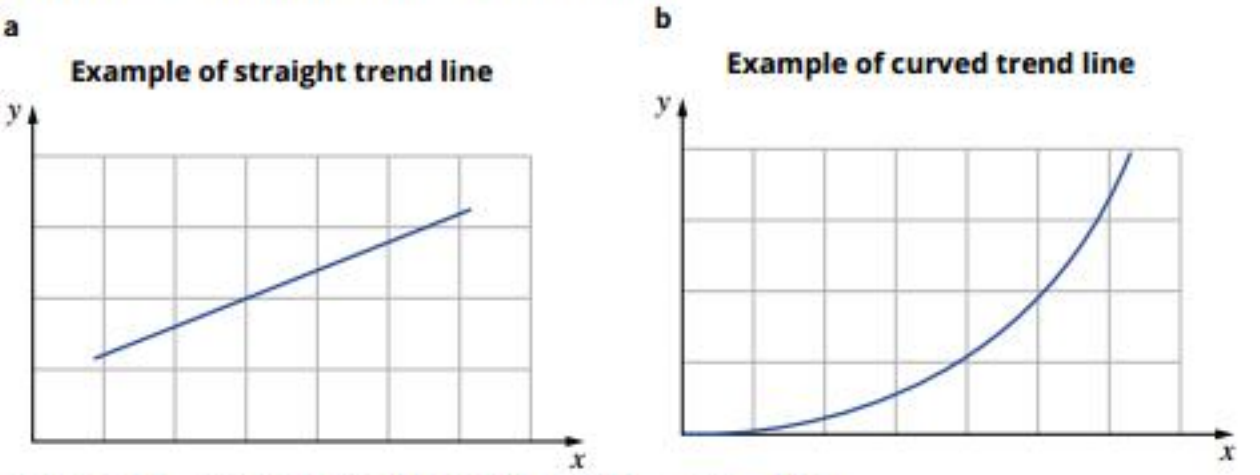


FIGURE 1.6.6 Graphs showing (a) straight and (b) curved trend lines.

Bar and column graphs

Bar and column graphs are used to show categories and **discrete (discontinuous) data**.

- A **column graph** shows the value of the dependent variable by the height of the column; the categories are labelled across the *x*-axis.
- A **bar graph** shows the value of the dependent variable by the length of the horizontal bar; the categories are labelled up the *y*-axis.

Bar and column graphs are commonly used when the independent variable is categorical rather than numerical, or when the numerical data is discrete. The bars or columns are always the same width and the same distance apart.

Bar and column graphs are very useful for graphing qualitative and discrete data, such as the water quality data from various locations along a waterway (Figure 1.6.7).

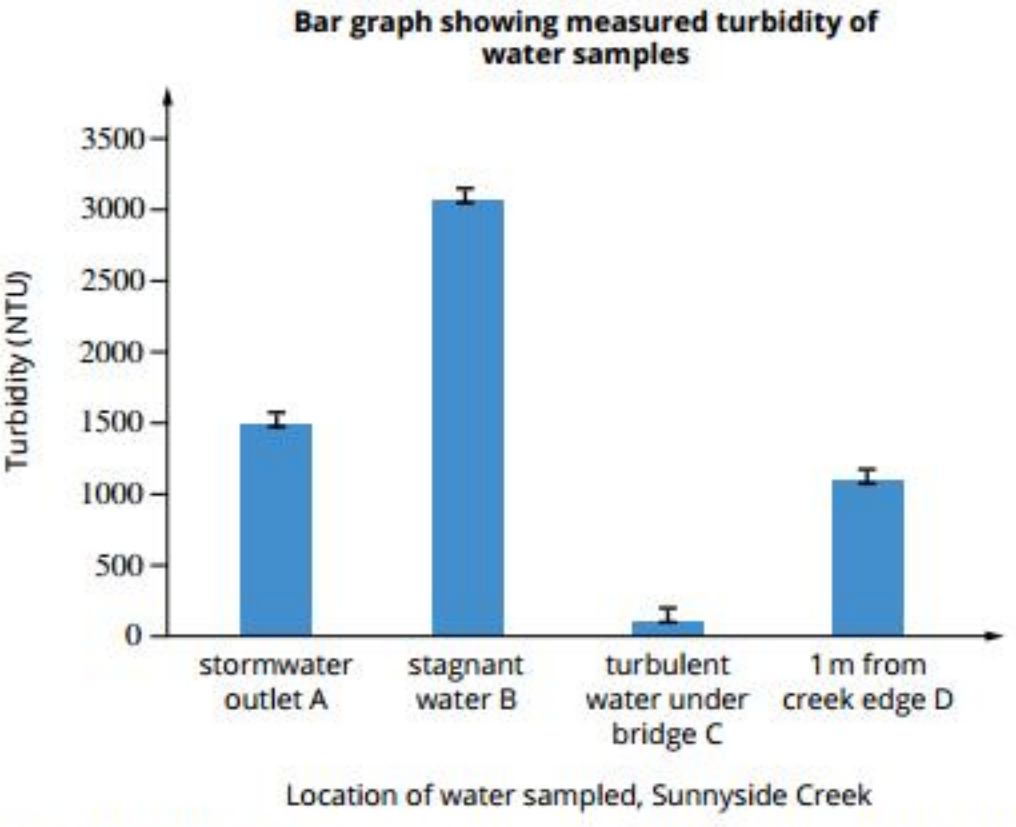


FIGURE 1.6.7 A column graph can be used to compare data. This graph shows the measured turbidity of water samples taken from various locations along Sunnyside Creek.

OTHER GRAPHING CONSIDERATIONS

Missing data

When you have missing data, leave a gap for it, as shown in Figure 1.6.8. Ensure that the axes are complete (do not skip values) and do not join the data points that have missing data points between them.

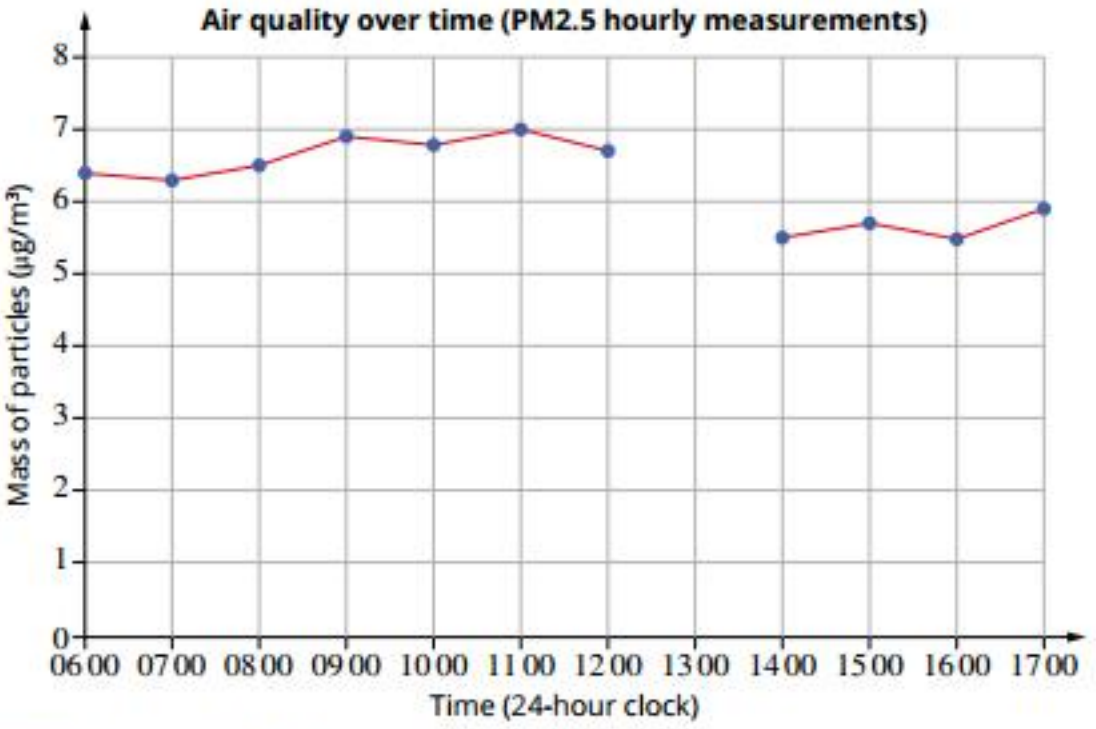


FIGURE 1.6.8 A line graph with data missing (for 1300).

Outliers

Sometimes when you collect data, there may be one point that does not fit the trend and may be an error. This is called an **outlier**. An outlier is often caused by a mistake made in measuring or recording data, or from a random error in the measuring equipment. This is covered in more detail later in this module. If you have an outlier in your results, you include it in your graph but ignore it when drawing the line of best fit, as in Figure 1.6.9 where the point (0.48, 0.08) is an outlier.

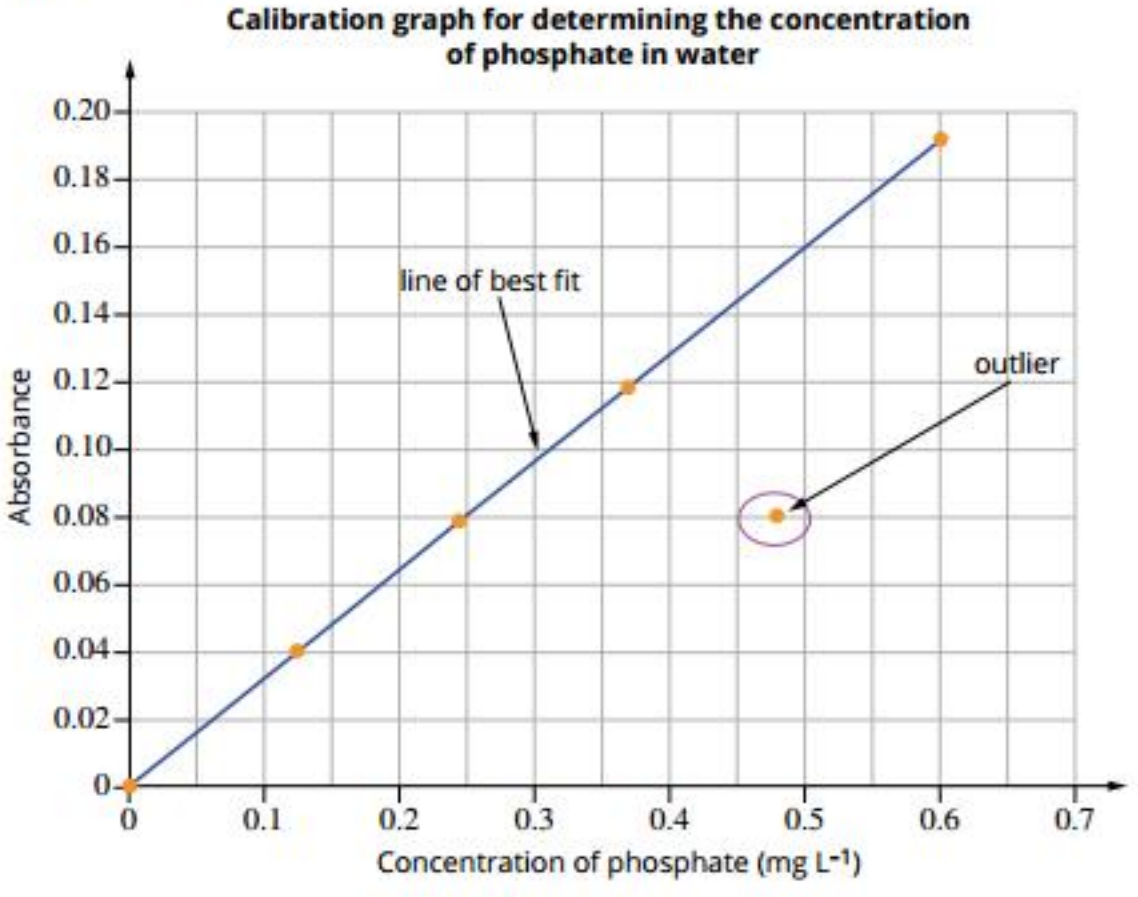


FIGURE 1.6.9 The graph is a calibration graph for determining the concentration of phosphate in water. A line graph shows an outlier, which has been ignored when adding the line of best fit.

Distorting the truth

Poorly constructed graphs can distort the truth. For example, in Figure 1.6.10, you can see two graphs that show the same data—the test results of two groups of students. One group of students did not eat breakfast before doing the test and scored an average of 42 marks out of 50. The other group of students did eat breakfast and scored an average of 48 marks out of 50. Figure 1.6.10b distorts the difference in marks between the two groups by using a scale of only 40 to 50 marks on the *y*-axis. It is important to make sure the graphs you create do not distort your data. You should also be wary of distorted data when interpreting graphs in other publications.

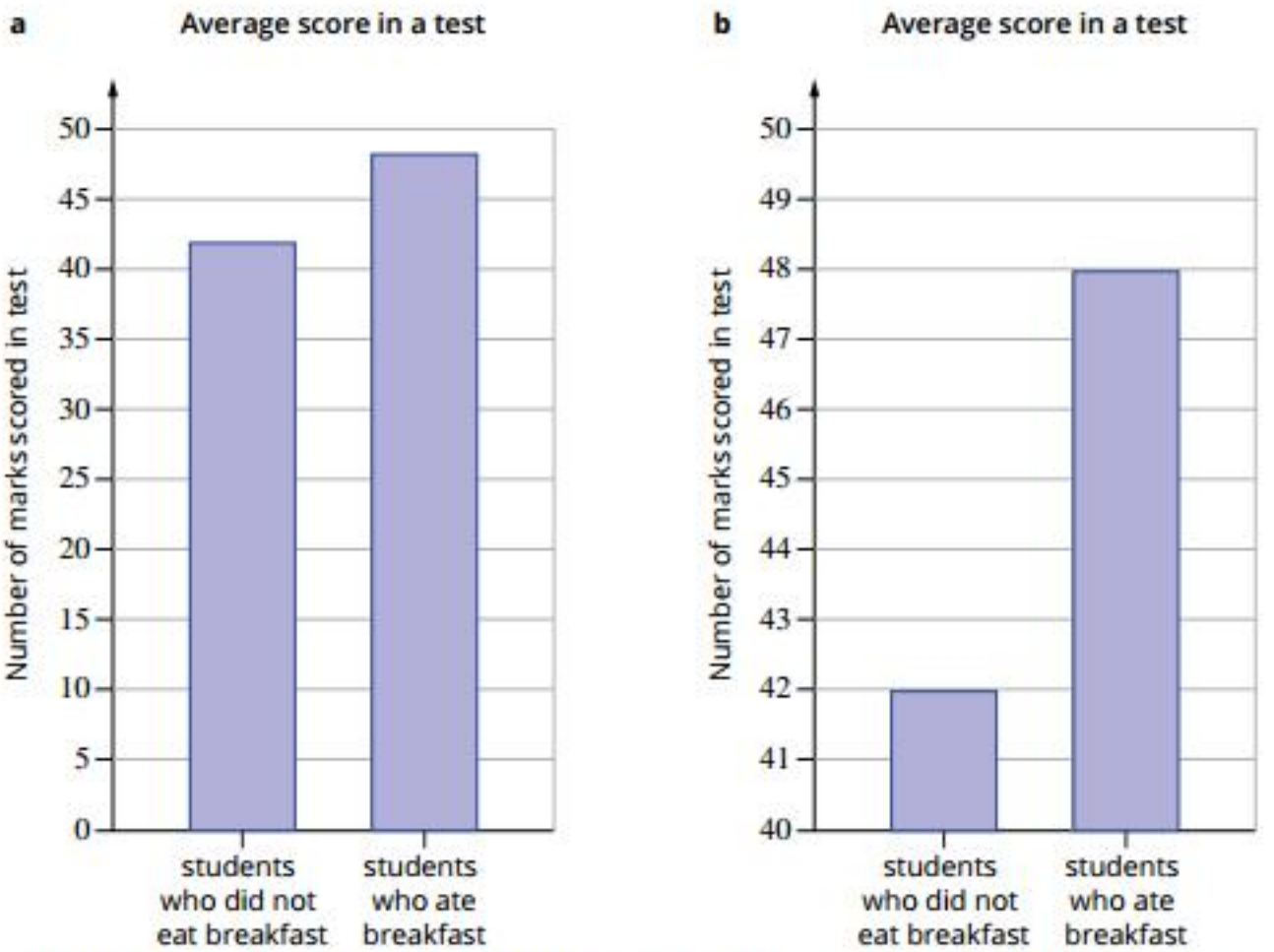


FIGURE 1.6.10 (a) shows the difference in the average scores between two groups of students (out of the maximum score of 50 marks) on the *y*-axis. (b) shows the difference between the two groups within only a narrow range of marks on the *y*-axis, which distorts the difference and makes it appear larger than it really is.

1.6 Review

SUMMARY

- Tables and graphs are used to represent scientific data.
- In general, tables provide more detailed data than graphs, but it is easier to observe trends and patterns in data in graph form than in table form.
- Tables organise data into rows and columns, and can vary in complexity according to the nature of your data.
- Tables should have the following features:
  - a descriptive title
  - column headings (including the units)
  - aligned figures (align the decimal points)
  - the independent variable placed in the left column
  - the dependent variable placed in the right column.
- Graphs are used to display relationships, trends and patterns between two variables with one proposed to be dependent on the other.
- There are several types of graphs, including line graphs and bar graphs. The best one to use will depend on the nature of the data.
- Scatterplots are commonly used to display data in the form of a graph, and can be used to plot raw or processed data.
- A trend line (line of best fit) is used to show the overall trend in the data, and can be used to predict values between the data points.
- A line graph is a good way of representing continuous quantitative data.
- Bar and column graphs are used to show categories and discrete (discontinuous) data.
  - A column graph shows the value of the dependent variable by the height of the column; the categories are labelled across the *x*-axis.
  - A bar graph shows the value of the dependent variable by the length of the horizontal bar; the categories are labelled up the *y*-axis.
- Missing data is represented in graphs by leaving a gap.
- An outlier is a data point that does not fit the trend, and may be caused by an error.

KEY QUESTIONS

Describe

1 State the purpose of a trend line.

Apply

2 Explain what outliers are.

3 Identify the relationship between the variables indicated by a sloping linear graph.

4 Explain how the general pattern (trend) of a graph can be represented once the points are plotted.

Analyse

5 Antonia draws a straight line graph of data, including error bars, from an experiment she has just completed. She finds that it is not possible to draw a straight line of best fit through every error bar. Analyse the problem and advise Antonia on what to do.

6 If a theory suggests that the *y*-intercept of a line is zero, deduce what this should look like on a linear graph.

7 Assess when it is more appropriate to use a graph showing a line of best fit rather than a ruled line graph that joins each point.

8 Consider the data below and determine the relationship between atmospheric pressure and altitude. Describe the trend and draw a graph, including a line of best fit.

Pressure (atm)	1.00	0.79	0.52	0.23	0.11	4.5×10^{-2}	1.3×10^{-2}	6.0×10^{-3}	2.1×10^{-3}
Altitude (km)	0	2.0	5.0	10.0	15.0	20.0	30.0	40.0	50.0

1.7 Data analysis

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- calculate and interpret the range, mean, median and mode of a set of data
- use the R^2 values to evaluate the fit of a trend to a set of data.

One of the difficulties in chemistry is that direct measurements of phenomena or measurements within a closed system are challenging to obtain. Therefore, the limitations and uncertainty in the data include uncertainties in the accuracy and precision of the measurements that were recorded, as well as errors related to reliability and validity of the experimental procedure. To address this problem, chemists perform statistical analysis to help understand the quality of the measurements, the results and their meaning.

This module will outline a basic understanding of common statistical analysis used in chemistry relevant to the Chemistry General Senior Syllabus.

STATISTICAL MEASURES

There are a number of common statistical measures that help describe data accurately.

Range

The range is the difference between the highest and lowest values in a data set. Table 1.7.1 shows the measurements taken for a reaction between sodium thiosulfate and sulfuric acid.

TABLE 1.7.1 Time for the reaction mixture to turn opaque in the reaction between sodium thiosulfate and sulfuric acid at 20°C and 50°C

Temperature	1	2	3	4	5	Mean	Range
20°C	253	158	201	169	187	187.6	253 – 158 = 95
50°C	69	85	70	91	75	78	91 – 69 = 22

To determine the range for values in Table 1.7.1, you would subtract the smallest value from the largest value. Notice how an abnormally large or abnormally small value in the data set makes the variability appear high. If one value appears way out of range, such as the time taken for the reaction mixture to turn opaque for the first time the reaction was performed at 20°C, it may be an outlier. This illustrates the importance of observation during experiments and recording all details in a journal as experimentation and research is conducted.

The experiment was conducted with a smaller number of measurements taken at each temperature, and the results are shown in Table 1.7.2.

TABLE 1.7.2 Time for the reaction mixture to turn opaque in the reaction between sodium thiosulfate and sulfuric acid at 20°C and 50°C

Temperature	1	2	3	Mean	Range
20°C	253	158	201	194	253 – 158 = 95
50°C	69	85	70	75	85 – 69 = 16

A larger **sample size** will strengthen the **validity** of the range.

Even though the range has not changed much between Tables 1.7.1 and 1.7.2, the results at 20°C seem more random. In Table 1.7.2 at 50°C, the second reaction could be an outlier as the other two results show excellent agreement. The range simply outlines the total variation in measured results; no other analysis or interpretation can be achieved.

Measures of central tendency

Measures of central tendency (also called central location) are single values that allow you to describe the central position in a set of data. The mean, median and mode are all measures of central tendency.

Consider the following data set: 3, 5, 7, 8, 8, 8, 10.

- The **mean** (or average) is the sum of the values divided by the number of values, which in this case is $(3 + 5 + 7 + 8 + 8 + 8 + 10) \div 7 = 7$.

$$\text{mean} = \frac{\sum(x_1 + x_2 + x_3 + \ldots)}{n}$$

where Σ = sum of

$x_1 + x_2 + x_3$ = measurement$_1$ + measurement$_2$ + measurement$_3$

n = total number of measurements

- The **median** is the 'middle' value in an ordered list of values, which in this case is the fourth value, which is 8.
- The **mode** is the value that occurs most often in a set of values, which in this case is 8. This measure is particularly useful for describing qualitative or discrete data.

The appropriate measure of central tendency to use depends on the type of data you are working with (Table 1.7.3).

TABLE 1.7.3 When to use the different measures of central tendency

Type of data	Mean	Median	Mode
nominal (qualitative)	✓	✗	✗
ordinal (qualitative)	✓	✓	maybe
discrete or continuous (quantitative)	✓	✓	✓

Graphically representing the data using central tendency provides a clear and succinct display of results. As there are many measured values and results in raw data, it can be difficult to analyse and interpret. It is much easier and less complicated to analyse and interpret processed data compared to raw data. Raw data includes all the measured results and usually a large number of measurements or observations.

Processed evidence is usually a smaller number of results that represent all the measured raw data; these representative results are calculated using statistical methods such as mean, median and mode. Therefore, an analysis can be conducted to compare fewer results (e.g. two means) rather than comparing all the individual measurements in a set of raw data. Interpreting a relationship between variables is also much easier and less complicated when using fewer numbers.

It is important to realise that statistical calculations do not produce the true value, but rather a single value (or smaller number of values) that is meant to represent many. Analyse the mass of two alcohols burnt in a calorimetry experiment, shown in Table 1.7.4. The average has been calculated for each alcohol; however, you will notice that the mean value was not measured during the experiment and is not in the raw data.

TABLE 1.7.4 Mass of ethanol and hexanol burnt

Ethanol (g)	Hexanol (g)
0.77	1.60
0.78	1.82
0.72	1.67
0.73	1.72
0.76	1.71
0.74	1.80
Mean 0.75	Mean 1.72

REGRESSION

Regression is the term used to describe the degree to which the independent variable causes the change in the dependent variable during a scientific investigation. Some relationships between variables are causal, meaning that there is a cause-and-effect relationship. The independent variable is the cause and the dependent variable is the effect.

There are numerous statistical calculations that estimate the causal relationship between variables. Some calculations provide a value that indicates how directly an independent variable causes the dependent variable result. This attempts to show the strength of the relationship, and to identify if the change in the dependent variable is entirely due to the independent variable.

In chemistry, not all relationships are direct or straightforward cause-and-effect. Often there are many variables that influence the dependent variable and it is helpful to try and predict how much of an effect the independent has on the dependent variable, even when other variables are also influential.

Coefficient of determination (R^2)

The **coefficient of determination** (R^2) produces a value that is an estimate as to how well you can predict the dependent variable based on the independent variable, considering the variations in the results. In the examples in Figure 1.7.1, the data for technique 1 does not follow the linear trend line exactly; therefore as the concentration changes (the independent variable), the absorbance (dependent variable) does not always change consistently. The coefficient of determination is a calculation that considers the variation in the results to estimate the predictability.

For example, a laboratory has used two different analytical techniques to determine the concentration of a performance-enhancing drug in a blood sample from an athlete suspected of cheating. The calibration curves for each technique and the R^2 value for each technique are shown in Figure 1.7.1.

Based on the lines of best fit and R^2 values, the second method was chosen to analyse the athlete's blood sample.

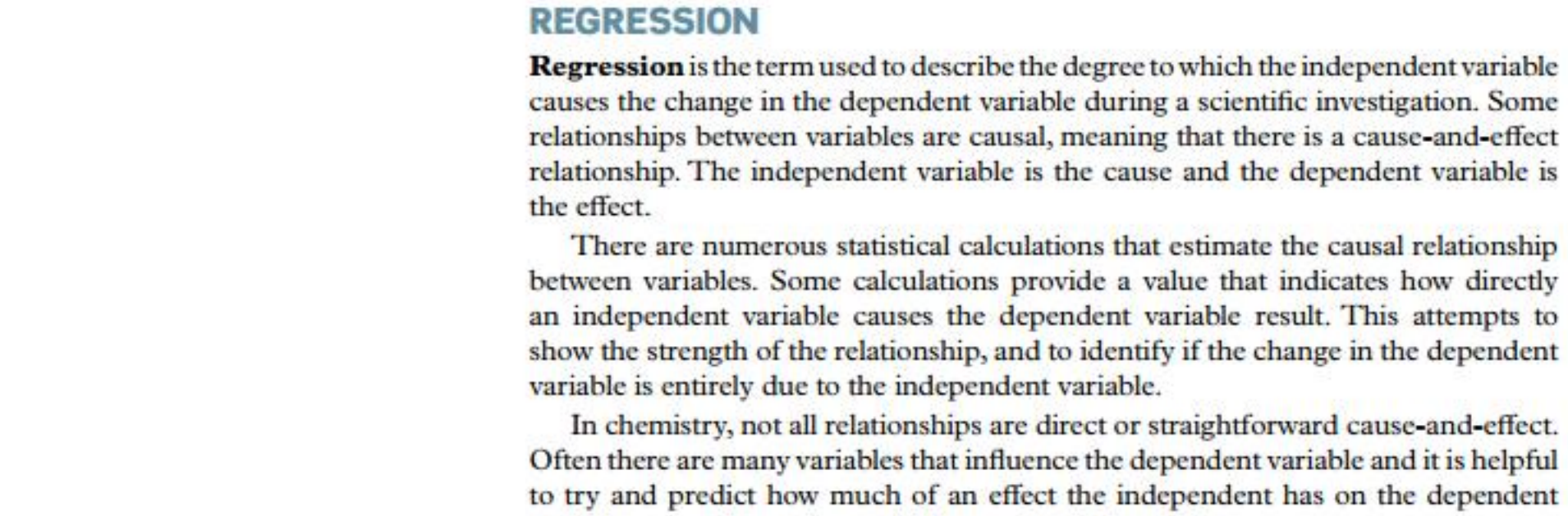


FIGURE 1.7.1 (a) The calibration curve for technique 1: Linear regression was used to establish a line of best fit. (b) The calibration curve for technique 2: Linear regression was used to establish a line of best fit.

Even though both techniques measured the same samples, the data is different. As can be seen in the graphs, the linear trend line has a similar slope; however, technique 1 has an R^2 value of 0.96 and for technique 2 it is 1.00.

The coefficient of determination produces a value between 0 and 1. If the value is 0, it is unable to predict the change in the dependent variable from the independent variable due to so much variation in the results. If the value is 1, then it can predict the change in the dependent variable 100% of the time without error. Any other number between 0 and 1 is considered a percentage, for example 0.76 means that the coefficient of determination can predict 76% of the dependent variable results due to change in the independent variable. It is interpreted as 76% of the variation in the dependent variable can be explained by the independent variable.

In Figure 1.7.1b, the absorbance of the sample was perfectly correlated without error with the concentration of the species. This suggests that the results from technique 2, including error, **bias** and instrumental precision, are highly reliable.

Figure 1.7.1a shows that the absorbance of the sample was not precisely correlated with the concentration. The R^2 value for technique 1 is lower than for technique 2, meaning the results are less predictable due to more variation. Technique 1 was less precise compared to technique 2; therefore, technique 2 is the preferred technique to determine the concentration in the actual sample.

1.7 Review

SUMMARY

- The range is the difference between the highest and lowest values in a data set.
- The mean, $\bar{x}$, is the average of a data set. It is calculated using the formula:
  $\bar{x} = \frac{\sum x_1 + x_2 + x_3 \ldots}{n}$, where
  $\sum$ = sum of
  $x_1 + x_2 + x_3$ = measurement$_1$ + measurement$_2$ + measurement$_3$
  n = total number of measurements.
- The median is the 'middle' value in an ordered list of values.
- The mode is the value that occurs most often in a data set. The mode is particularly useful for describing qualitative or discrete data.
- Regression is the term used to describe the degree to which the independent variable causes the change in the dependent variable during an experiment.
- Linear regression is a calculation that estimates a direct linear relationship between the independent and dependent variables.
- The coefficient of determination estimates how well you can predict the dependent variable based on the change in the independent variable.
- The coefficient of determination produces an R^2 value between 0 and 1.
  - The closer the R^2 value is to 0, the less predictable the dependent result is based on the independent value.
  - The closer the R^2 value is to 1, the more predictable the dependent result is based on the independent value.

KEY QUESTIONS

Describe

1 Define the terms 'mean', 'median' and 'mode'.

Apply

2 Explain why a coefficient of determination, R^2, cannot be greater than 1.

Analyse

3 For the data set {21, 28, 19, 19, 25, 24, 20}, calculate the:
- **a** range
- **b** median
- **c** mode
- **d** mean

4 Identify which of the statistical measurements of mean, mode and median is generally most affected by an outlier.

1.8 Scientific writing

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- use scientific language and representations
- use a scientific journal for experiments
- reference sources and avoid plagiarism
- use and reference AI in research and writing
- communicate findings in a multimodal presentation

The QCAA requires students to complete a student experiment as part of Unit 3 Chemistry and a research investigation in Unit 4 Chemistry. In preparation for Units 3 and 4, teachers may choose to assign similar assessment tasks in Units 1 and 2. Both tasks require written or multimodal presentations. Preparing and presenting scientific reports and investigations involves research and note-taking skills, use of scientific genre, language and representations and referencing knowledge to acknowledge sources used.

Scientists follow strict genre conventions when undertaking and communicating their work. These are described in this module. Refer back to this module as you complete the student experiment and research investigation.

SCIENTIFIC WRITING AND REPRESENTATIONS

Scientific reports must be written using scientific language and representations—these should be relevant, fluent and concise. To meet the word count or time requirements, only use the words required to communicate your information and avoiding repetition (Figure 1.8.1). Having a plan and using a journal also helps to achieve fluent and concise writing. Use the syllabus objectives, specifications and the instrument-specific marking guide (ISMG) to plan an outline of each section of your written task.

Table 1.8.1 demonstrates communication of the same concept in a few different ways. Being fluent and concise will significantly influence the word count of the report and the quality of the writing.

TABLE 1.8.1 Communicating concepts in various ways

Concept	Communication	Commentary of communication
the basic structure of an atom	An atom is made up of protons, neutrons and electrons.	This is fluent and concise, but lacks scientific terms or language to convey in-depth understanding.
	Atoms are tiny little objects made up of numerous parts that form the basis of matter. Atoms are made up of electrons, neutrons and protons. The electrons are found away from the centre of the atom. The centre of the atom contains the protons and neutrons.	This is fluent, but not concise. There is repetition (e.g. 'tiny' and 'little'—these terms have the same meaning; also 'made up' is stated twice). It also uses many words without using scientific terms to provide detail and understanding. This may be useful language in the journal when learning about a topic, but not in the scientific report.
	Atoms are particles composed of three types of subatomic particles: the proton, electron and neutron. The centre of an atom is the nucleus and contains the protons and neutrons, with the electrons occupying space external to the nucleus.	This is fluent and concise. Much in-depth understanding is communicated through scientific terms, which enable much information to be conveyed in fewer words.

Reports are written using paragraphs, with each paragraph explaining only one idea. The first sentence (topic sentence) of the paragraph introduces the topic. Following sentences provide the details of the idea. The final sentence concludes the idea and may also link to the idea of the next paragraph. Each sentence should flow onto the next, slowly building the details of the explanation.

Reports should be written using:

- past tense—as the experiment was conducted in the past, the report should be in the past tense
- third person, passive voice and impersonal verbs—science uses this language convention (Table 1.8.2)
- scientific language—the terms used are specific to concepts, models and theories
- information from secondary sources which is written in your own words
- objective, unbiased language—avoid subjective and emotional or persuasive writing (Table 1.8.3)
- concise language—avoid unnecessary repetition and express ideas. Scientific language allows more details, knowledge and understanding to be communicated in fewer words. Use shorter sentences that are less wordy. (Table 1.8.4)
- headings and subheadings can be used to break up a report

Table 1.8.2 shows some examples of more concise wording.

TABLE 1.8.2 Examples of first-person and third-person narrative

First person	Third person
I put 50 g of marble chips in a conical flask and then added 10 mL of 2 M hydrochloric acid.	*First, 50 g of marble chips was weighed into the conical flask and then 10 mL of 2 M hydrochloric acid was added.*
After I observed the reaction, I found that ...	*After the reaction was completed, the results showed ...*
My colleagues and I found ...	*Researchers found ...*

TABLE 1.8.3 Persuasive writing versus scientific writing styles

Persuasive writing examples	Scientific writing equivalent examples
Biased and subjective language: *The results are extremely bad/atrocious/ wonderful etc.* *This is terrible because ...* *This produced a disgusting odour.* *Health crisis!*	Unbiased and objective language: *The results showed ...* *The implications of these results suggest ...* *The results imply ...* *This produced a pungent odour.* *Health issue*
Exaggeration: *The object weighed a colossal amount, like an elephant.*	Non-emotive language: *The object weighed 256 kg.*
Use of everyday or colloquial language: *The bacteria passed away.* *The results don't ...* *The researchers had a sneaking suspicion ...*	Use of formal language: *The bacteria died.* *The results do not ...* *The researchers predicted/hypothesised/ theorised ...*

TABLE 1.8.4 Examples of verbose and concise writing

Verbose writing	Concise writing
Due to the fact that ...	*Because ...*
Smith undertook an investigation into ...	*Smith investigated ...*
It is possible that the cause could be ...	*The cause may be ...*
end result ...	*result ...*
In the event that ...	*If ...*
shorter in length ...	*shorter ...*

To produce a fluent report, the scientific language must be used without error so that the reader understands the meaning of the information easily. Refer to the syllabus for the correct scientific terminology. For the report to be concise, there should not be any repetition. Being fluent and concise will significantly influence the word count and the quality of writing. Refer to the syllabus ISMG to identify the cognitive verbs used in the descriptors to produce the appropriate response. For example, you will need to write more extensively if you are asked to 'discuss' or 'explain' compared to 'identify'.

Scientific representations

Chemical structures, equations and diagrams are an efficient way of presenting complex data and explaining chemical concepts. Flow charts, graphs, tables and photographs are also used. Ensure you include:

- a descriptive title
- labels, captions or descriptions
- numbering; for example, Figure 1, Figure 2 etc. or Table 1, Table 2 etc.
- a source if the work is not your own or is adapted from work that is not your own.

SCIENCE JOURNAL

There is a lot of information to record during the student experiment or research investigation, so it would be best to keep a **scientific journal**. Entries in your journal should include the following features:

- the date of entry
- ideas, observations, proposals, questions
- background information you researched for the task
- new terms and definitions
- refinements
- results, data, evidence, variables
- explanations, ideas, observations (including diagrams)
- limitations, conclusions, further investigation

A journal holds a record of information used during the process of the scientific method (Figure 1.8.1). You will not know what is vital information until your experiment is complete and summarised into the scientific report. Data and graphs may be saved digitally, so reproduce a sketch in your journal that you can annotate with your thoughts. You may choose to prepare a page or two each for the four key sections of the task (e.g. for IA2; Forming, Finding, Analysing, Interpreting and Evaluating) or use proposed report headings (e.g. Rationale, Research Question etc.).

Researched and recorded information in your journal will be used for the Rationale, to justify the modifications to the methodology, to provide a reason for collecting data, to inform risk, ethical and environmental management, and to collate and process the data. It will also inform the interpretation of the evidence (results) and conclusion. Remember, parts of the Rationale (planning) and the data collection are completed with your group and shared—the rest of the task is individual and so is your journal. A journal is not an assessed part of the task but will likely be reviewed by your teacher as a progress check and to confirm the work is yours. Depending on the size of the journal, it may be copied and attached in the Appendix of your report.

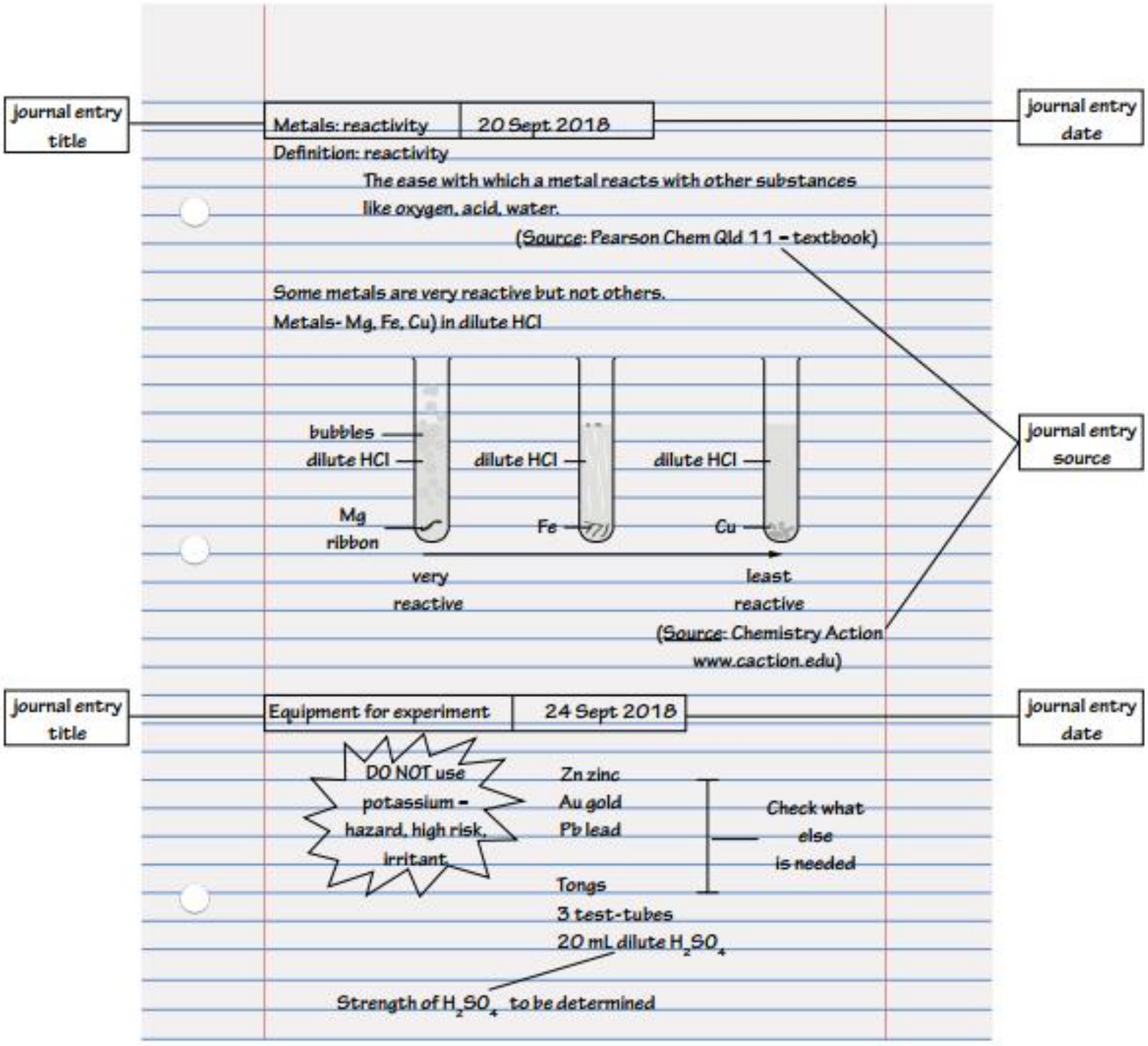
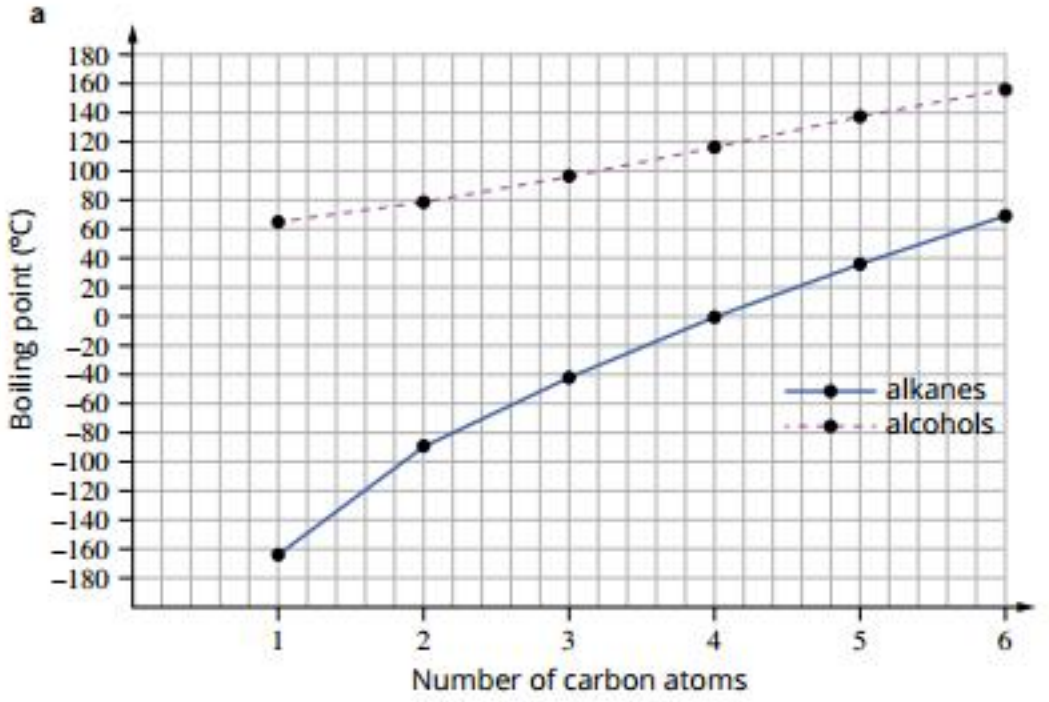


FIGURE 1.8.1 A journal entry with the journal entry date, titles and apparatus used in preparation for an experiment. There will be numerous journal entries on any given date, and they should have their own titles. Also, the same titles will appear on different entry dates as research continues on specific topics.

Journal entries can take different formats. Sometimes one form of recording information provides more details than others. Note taking is not limited to words. Figure 1.8.2 presents the same information in different ways.

a



b

The boiling points increase with increasing number of carbon atoms. This indicates that the intermolecular forces that are being broken during boiling are getting stronger.

The intermolecular bonds between alcohol molecules are stronger than the alkane molecules that contain the same number of carbon atoms.

The difference in electronegativities between the oxygen and hydrogen atoms creates a polar bond which means that the intermolecular bonds are stronger-forms H bonds compared to the temporary dipoles in alkanes, as the electronegativities of carbon and hydrogen atoms is much less.

The gap between each line is decreasing.

c

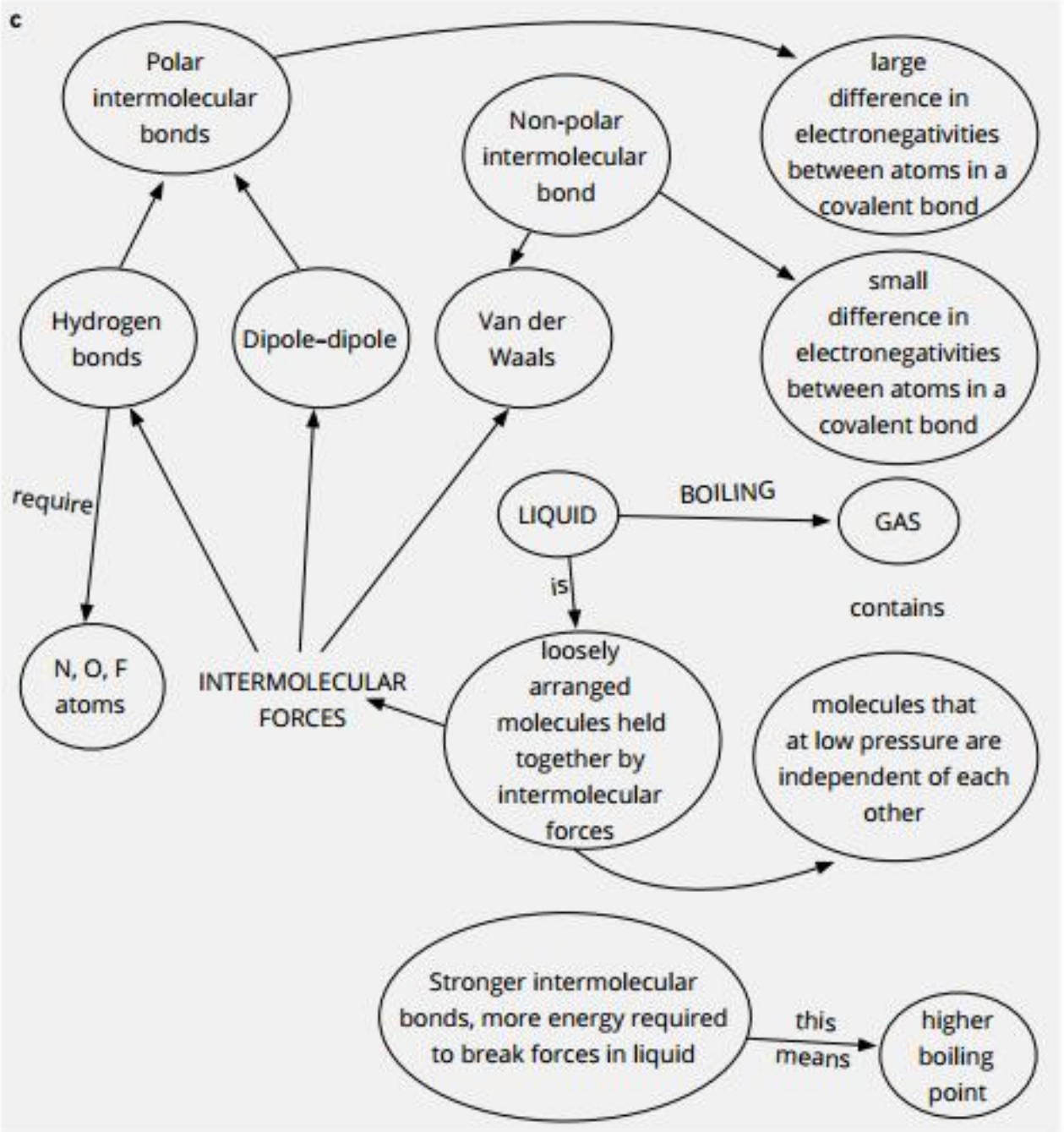
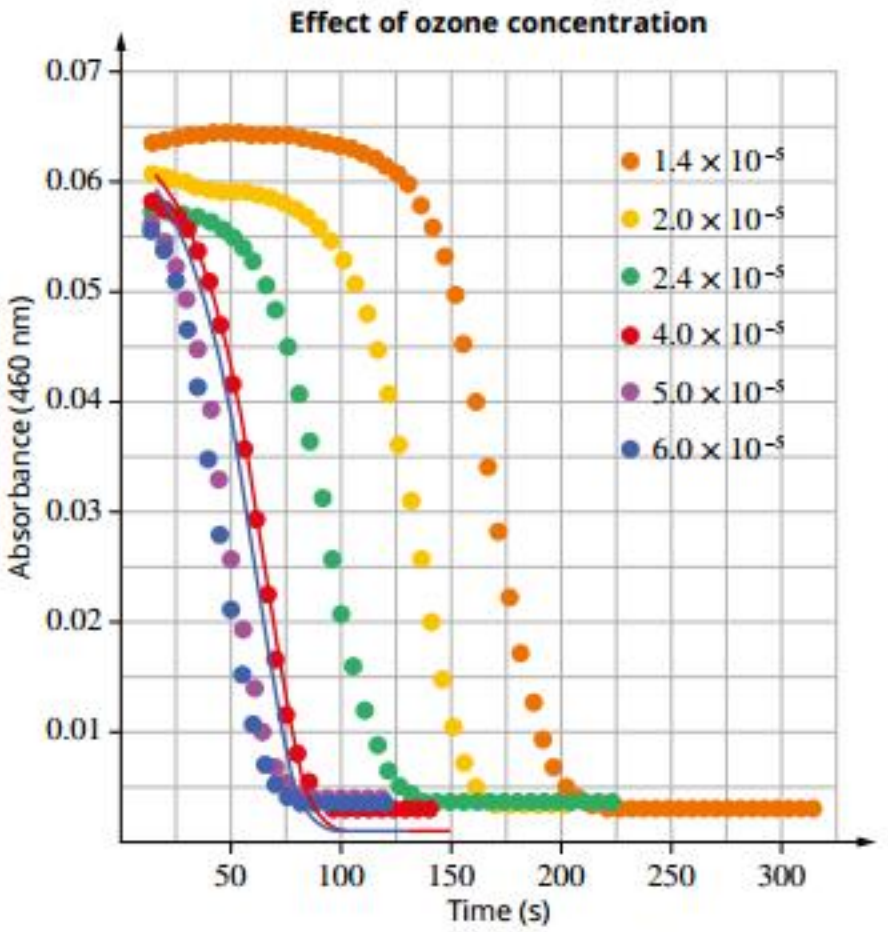


FIGURE 1.8.2 (a) Graphical representation of the boiling point trend for alcohols and chain alkanes. (b) Written comparison of the boiling point trend. (c) Concept map linking electronegativities of atoms to the boiling points.

When recording results, data or evidence in your journal, be critical and interpret the data as it is collected. In this way, errors in the method are identified or sample size can be adjusted, if needed. If a given group member has the recording task, it is vital that the dataset is passed to all group members before leaving the laboratory. Add this information directly into your journal and annotate with your own comments. Figure 1.8.3 shows an example of research evidence and how it is interpreted in a journal. Notes in your journal can also include:

- specific details and your interpretation of significant values
- the trend or pattern and a statement of whether this is the expected one
- the comparison or difference between one set of values and another
- the statistics used to establish the significance and the author's interpretation.



Effect of the ozone concentration on the clock time.
The initial concentrations after mixing the reactants in the cuvette were as follows:
$[O_3]$ as indicated in the figure (mol L^{-1}),
$[NaClO_3] = 0.0251$ mol L^{-1},
$[HClO_4] = 0.474$ mol L^{-1}, and
$[I_2] = 8.8 \times 10^{-5}$ mol L^{-1}.
Experimental data (symbols); modelling results (continuous line).

FIGURE 1.8.3 Example of interpretation of research evidence.

REFERENCING SOURCES

When gathering scientific evidence for a scientific inquiry such as your student experiment and research investigation, source it from reputable publications such as:

- your textbook and practical manual. This should be your first source of reliable information.
- scientific journals and magazines: research papers and scientific reviews. Common commercial science magazines that you might find in your school library include *The Helix*, *Cosmos*, *Scientific American* and *New Scientist*. Scientific journals are peer-reviewed which gives them credibility.
- podcasts and websites. Electronic sources include online scientific organisations such as CSIRO, NCBI, AIMS, Bioscience (Oxford Academic) and other university publications and press. In general, use websites that are .edu, .gov or .org. Many government and privately funded science organisations publish useful material, along with not-for-profit scientific organisations. Websites may direct you to magazines and scientific journals, podcasts, blogs and videos.

In the syllabus, you are asked to "discuss and evaluate the validity and reliability of evidence" (Science Inquiry skills). When selecting and using sources of information and evidence, follow these guidelines:

1 Confirm that it is relevant.
   - **a** Check that it contains information that is specifically related to the inquiry.
   - **b** Check that the evidence and information are pertinent to the variables of the inquiry.

2 Assess its reliability.
   - **a** Is it current/recent information?
   - **b** Is it correct in its understanding of relationships?
   - **c** Is the evidence in agreement with other sources?
   - **d** Check credibility and bias—consider who the author is, their qualifications, expertise and affiliations.
   - **e** Evaluate the methodology, including what variables were controlled or measured.

It is not necessary that each of your sources fulfil all of these requirements. Each source will have strong and weak points. For example, we are confident that information from a peer-reviewed scientific journal is unlikely to lack credibility or contain bias because the review process is undertaken by experts in the field. However, it may have been produced 10 years ago and so scientific information and relationships may not be up-to-date. Also, podcasts or science magazines for school students may contain a wide array of interesting real-world examples but may not explain the scientific understandings in sufficient detail. Some resources are available by paid subscription, so use advice from your school librarian about free resources or join your local library.

All quotations, documents, publications and ideas used in your investigation need to be acknowledged in the reference list in order to avoid plagiarism and to ensure creators are properly credited for their work. When using sources to explain chemical concepts or review data, ideas must be written in your own words (see plagiarism, below). References and acknowledgements show that you have read widely, give credibility to your study and allow the reader to locate information sources should they wish to study it further.

Plagiarism

Plagiarism is using other people's work without acknowledging them as the author or creator. To avoid plagiarism, include a reference every time you report the work of others; for example, at the end of a sentence or following a diagram. If you use a direct quotation from a source, enclose it in quotation marks. This will ensure you give credit to the original author and it will enable the reader to find the original source.

Information taken from a source should be rewritten in your own words. It can be difficult to reword information in your own words. A useful strategy is to read the information, understand it, then, without looking back at the source, take notes in your journal. Notes that are detailed and have full explanations will be useful when you refer to them later to write the report.

TABLE 1.8.5 Suggestions for rewording information

Source information:	
"It can be expected that the days will be warm and the nights will be cool over the next three days due to the high pressure system moving across the region."	
Strategy to change source information	**Reworded information**
The order of information can be swapped—the object (the warm days and cool nights) with the reason (high pressure system).	Due to the high pressure system moving across the region, the days will be warm and the nights will be cool.
Some words can be changed such as adverbs, nouns, verbs, adjectives.	It has been predicted that during the daytime it will be warm while the evenings will be cool for about three days, as a high pressure system travels over the region.
Information can be elaborated to explicitly outline information.	The weather forecast expects (or, made a prediction based on computer simulations) that the temperature during the day will be warm (22–25°C) and the evenings will be cool (below 12°C) due the high pressure system (or, weak high pressure system), which dissipates clouds and allows direct sunshine to warm the Earth's surface; however, in the evenings this system brings cool air from higher altitudes, which is no longer warmed by the sun.

Referencing

There are a number of different referencing styles, such as Harvard or APA. The sources of information must be acknowledged using a referencing style that is suitable for the purpose of the investigation. Check the preferred referencing style or convention of your teacher for in-text referencing and a complete a **reference list**. APA (American Psychological Association) style is the most commonly used referencing style. Reference examples are shown in Table 1.8.6.

A bibliography is a list of all the sources used during the research to develop understanding (including information in the journal) even if the information was not used directly or explicitly in the scientific report. A reference list only lists the sources used and cited (or in-text referenced) in the scientific report. As such, a reference list is the minimum requirement and you may choose to extend this to a bibliography. The sources must be listed at the end of the report in the style consistent with your style of referencing.

Compile all references you use both directly in the scientific report or in the gathering and development of the information in a separate document as you conduct the investigation. This will save you time later. Microsoft Word and other online tools make writing a reference list easier by automatically formatting references in the referencing style of your choice. Always check that this tool has formatted correctly.

TABLE 1.8.6 Examples of references

Books	Author surname then initials, year of publication, title, publisher,	Yurkanis Bruice, P. (2024), *Organic Chemistry*, Pearson (one author) Natu, A. D., Bobade, V. D., & Gugale, G. S. (2019), *Organic Chemistry*, Nirali Prakashan (more than one author)

In-text citations

Each time you write about the findings of other people or organisations, you need to provide an in-text citation and provide full details of the source in a reference list. In the APA style, in-text citations include the first author's last name and date in brackets (author, date).

The following example shows two types of in-text citation and the reference list entry.

In-text citations
It was reported that in testing of five pro-oxidant additives added to commonly manufactured polymers, none resulted in significant biodegradation after three years (Selke et al., 2015).
Selke et al. (2015) reported that in testing of five pro-oxidant additives added to commonly manufactured polymers, none resulted in significant biodegradation after three years.
Reference list entry for the example above would be:
Selke, S., Auras, R., Nguyen, T. A., Aguirre, E. C., Cheruvathur, R., & Liu, Y. (2015), Evaluation of biodegradation—promoting additives for plastics. *Environmental Science & Technology*, 49(6), 3769–3777.

USING AI IN RESEARCH AND WRITING

Generative AI (or just AI) uses chatbots or digital assistants that you can communicate with using fairly natural language to access information in Large Language Models (computer models trained on vast amounts of data). These typically generate text, and some models can generate images, video and audio.

AI can be great for brainstorming ideas about investigations, generating practice questions and generating data for investigations. However, you must follow guidance from your teacher or school on how you can use AI in your work. You could be penalised by your school for using AI-generated material without permission or acknowledgement. It's also important to understand the limitations of AI-generated text.

- Check with your teacher before using AI in your work.
- Acknowledge use of AI using referencing conventions.
- Always fact check AI-generated text and references.

Limitations of AI-generated text

Large language models are engineered to match patterns of words, but they can't understand the meaning of your prompt or the output text. They produce text that is similar to patterns of words in the prompts and outputs they have been trained on. This can result in text that sounds knowledgeable and authoritative but does not mean much when you examine it or try to rephrase it in simple language. AI can hallucinate—i.e. make up statements—and this can be obvious or subtle. For example, AI can give correct answers to questions it has generated but give the wrong explanations.

The data that the model is trained on is not necessarily scientifically accurate, so generated text could be incorrect or biased. AI can be prompted to provide references, but these are often not reliable.

AI-generated answers may not model the complete response that aligns with the scope and scale of the syllabus. In class, you will have developed an understanding of the scientific concepts described in the syllabus. In this way, you can check the level of information and accuracy provided in an AI-generated response.

Referencing AI sources

You must properly acknowledge the use of AI in your work. Some AI tools provide a URL that will link to generated text. If yours does not, it's a good idea to include the prompt you used and the AI output as an appendix to your work. The following are sample ways to reference AI-generated text (Table 1.8.7).

TABLE 1.8.7 Examples of ways to reference AI-generated text

Referencing style	General format	Example
APA	Author. (Year). Title of software program (Version). Date. URL. Appendix.	OpenAI. (2024). *GPT-4o*. 20 June 2024. URL or 'see Appendix for prompt used and output generated'.
Chicago	Footnote number. AI tool used, Month Day, Year, Creator of tool, URL, Appendix.	1. Text generated using GPT-4o, June 20, 2024, OpenAI, URL or 'see Appendix for prompt used and output generated'.

Prompting the digital assistant

Learning to write effective prompts is essential to get good results from AI. There is no perfect way to write a prompt, but using one of the many frameworks can be useful. Keep the instructions simple—for example:

- Role (Who the chat assistant is being: e.g. policy maker, marketer, consumer)
- Task (What output you would like: e.g. an article, summary, set of questions)
- Format (What it should look like: e.g. bulleted list, table, graph)

For example: I am a government policy maker working on energy strategy. Give me a one-page summary of pros and cons of using nuclear power in Australia. Consider cost, climate change, security, the environment and First Nations' perspectives in your answer. Present the summary in bullet points and include accurate references for all data.

If necessary, you can refine the results using further prompts. Note that chat assistants are not predictable, and you can get different results using the same prompt.

MULTIMODAL PRESENTATIONS

Student experiments and research investigations are focused investigations resulting in a conclusion related to the initial question posed. In schools, the process occurs over a number of lessons but in research science, a project can continue for weeks, months or years. The reporting of the final findings is usually a written report published in a scientific journal but can also take place at a scientific conference. In the Queensland Chemistry syllabus, you are also provided this flexibility in the form of multimodal presentation as an alternative to the written report.

It is important to note that this mode gives you an option for the final presentation of the task only. All criteria and descriptors in the ISMG relating to forming, finding, analysing and interpreting/evaluating need to be met as described in Parts B and C. Multimodal presentations must include at least two modes of delivery at the same time, have a maximum time of 11 minutes and maximum 2000 words. Your two modes are likely to be visual (PowerPoint or poster) and verbal (speech). For average speaking speed, 11 minutes will equate to around 1600–1700 words. Your teacher will need the PowerPoint printed and a printed script—they may record your presentation. Another option is to use the audio record function of PowerPoint. These aspects of assessment will be identified by the school on their endorsed task(s).

Some considerations regarding the speech are:

- engage and effectively communicate with the audience
- use a clear structure—it is suggested to follow the outline of a written report (see headings provided in Parts B and C)
- interact with your PowerPoint or poster to point out important aspects
- while it is not advisable to speak on a tangent or set up a conversation with the audience, it would be possible to ask the audience if they have any questions
- use a strong confident tone
- bring your own timer to avoid going over time.

Some considerations regarding the visual presentation (for PowerPoint):

- each slide should have a clear focus with minimal text (6–7 lines per slide, 6–7 words per line). Use minimum 24 font size so that audience can read
- present a single graph or table per slide. For graph axes or annotations in smaller font, you should read out the information
- use a consistent design or theme.

Some considerations regarding the visual presentation (for poster):

- use a presentation size large enough to include all your graphs, figures and text
- make the poster 'flow' so the reader clearly follows the investigation from planning through to concluding and evaluating
- allow your audience some time before the presentation to view the information and allow them to formulate questions.

Communicating experimental or research findings is an integral part of a scientist's work. Irrespective of the time span of the investigation, there is a sense of achievement when the results are made known, especially when the process requires you to relate to the topic in depth. By choosing a verbal presentation, you can share this journey with the audience.

1.8 Review

SUMMARY

- Scientific reports use scientific language and representations.
- The language of scientific reports is concise, objective and written in the third person.
- The scientific visual representations include tables, charts, graphs, tables, illustrations.
- Visual representations include headings, labels, captions, descriptions, and numbering (if more than one item).
- A science journal is a useful tool for recording detailed information and sources during an investigation.
- Write using your own words to avoid plagiarism.
- Acknowledge sources and any references to the work of others by including a reference list.
- If using AI for scientific research, ensure information is checked against other sources, avoid plagiarism and acknowledge the source.
- A written or multimodal format may be used for your report but the same syllabus criteria and descriptors apply to both formats.

KEY QUESTIONS

Describe

1 Explain the difference between a bibliography and a reference list.

2 Describe what plagiarism is and indicate why it is unacceptable.

PART B STUDENT EXPERIMENT

The student experiment requires you to undertake the full **scientific method**. The Queensland Chemistry General Senior Syllabus 2025 states that this process begins with a practical conducted during class or viewed online. This practical will be modified to conduct your own experiment. It is recommended that during the class practical you record your observations, queries and thoughts as well as collect and process data. These notes can be used to develop a research question for the student experiment. This task assesses syllabus objectives, science inquiry skills and relates to student experiment objectives and specifications from the Chemistry General Senior Syllabus 2025. The student experiment constitutes 20% of the total assessment and may be presented in:

- written form (e.g. scientific report), up to 2000 words, or
- multimodal presentation form (at least two modes delivered at the same time), up to 11 minutes.

In the modules that follow, you will find a guide to a scientific method and an outline for producing a report of the student experiment.

INSTRUMENT-SPECIFIC MARKING GUIDE

Student responses are assessed against an instrument-specific marking guide (ISMG). In developing your experiment and planning your response, it is important to always have in mind the assessment objectives, and in particular the characteristics that are described in the performance level descriptors.

- The ISMG has four criteria (criterion): forming, finding, analysing, and interpreting and evaluating.
- Criteria have performance levels, against which the qualities of the response are assessed. The table below shows the high performance level characteristics for the four criteria.
- A performance level consists of a performance level descriptor and performance level mark or mark range.
- The performance level descriptor describes the characteristics that are demonstrated by a response at this quality.
- The ISMG criteria, and elaborations of each are shown in Table A, for the highest performances.

TABLE A Alignment of syllabus criteria, objectives, descriptors and marks with the modules of Part B

Criteria	Assessment objectives	Instrument specific marking guide (ISMG) – Criteria are demonstrated by:	Marks	Module
Forming	1. Describe ideas and experimental findings about chemical equilibrium systems or oxidation and reduction. 2. Apply understanding of chemical equilibrium systems or oxidation and reduction to modify experimental methodologies and process data. 6. Investigate phenomena associated with chemical equilibrium systems or oxidation and reduction through an experiment.	• a considered rationale for the experiment • justified modifications to the methodology • a specific and relevant research question • a methodology that enables the collection of sufficient and relevant data • appropriate use of genre and referencing conventions	5	1.9 1.8
Finding	1. Describe ideas and experimental findings about chemical equilibrium systems or oxidation and reduction. 6. Investigate phenomena associated with chemical equilibrium systems or oxidation and reduction through an experiment.	• considered management of risks/ethical issues/ environmental issues • collection of sufficient and relevant raw data • fluent and concise use of scientific language and representations	5	1.10 1.8
Analysing	2. Apply understanding of chemical equilibrium systems or oxidation and reduction to modify experimental methodologies and process data. 3. Analyse experimental data about chemical equilibrium systems or oxidation and reduction.	• correct and relevant processing of data • thorough identification of relevant trends/ patterns/relationships • thorough and appropriate identification of the uncertainty and limitations of evidence	5	1.11

Criteria	Assessment objectives	Instrument specific marking guide (ISMG) – Criteria are demonstrated by:	Marks	Module
Interpreting and Evaluating	4. Interpret experimental evidence about chemical equilibrium systems or oxidation and reduction. 5. Evaluate experimental processes and conclusions about chemical equilibrium systems or oxidation and reduction.	• justified conclusion/s linked to the research question • justified discussion of the reliability and validity of the experimental process • suggested improvements and extensions to the experiment that are logically derived from the analysis of evidence	5	1.12
Total			20	

The final report for the student experiment may be organised under the criteria headings in the ISMG: Forming, Finding, Analysing and Interpreting and Evaluating. However, this is not mandated, and you may elect to organise your report in a different but logical order using alternate headings.

Note that items in the appendix, reference list and in-text references are not included in the word count. The contents of the appendix are not used for determining levels of achievement.

The headings and sub-headings in Table B show one possible structure of a student experiment report (*alternate positioning of Conclusion section):

TABLE B Possible student experiment structure. Two possible positions for the conclusion.

Forming	Rationale
	Research question
	Modifications
Finding	Risk assessment
	Raw data
Analysing	Sample calculations
	Processed data
	Analysis
Interpreting and evaluating	Conclusion*
	Evaluation of experimental process (reliability and validity)
	Improvements and extensions
	Conclusion*
	Reference list/Bibliography
	Appendix

1.9 Forming

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand how to identify and modify an experimental investigation
- be able to research relevant background information that informs the research question
- develop the investigation by forming a research question which includes specific variables
- justify modifications to the original experiment

RATIONALE

Your student experiment uses a completed class practical or simulation as a basis for further experimentation. This means that the rationale will show an idea flow which begins with an original experimental result and uses scientific reasoning to propose a new and related question (Figure 1.9.1). Often, the same or similar experimental apparatus is used but independent and/or dependent variable(s) are altered. Conversely, a new experimental design and equipment is used to investigate the topic.

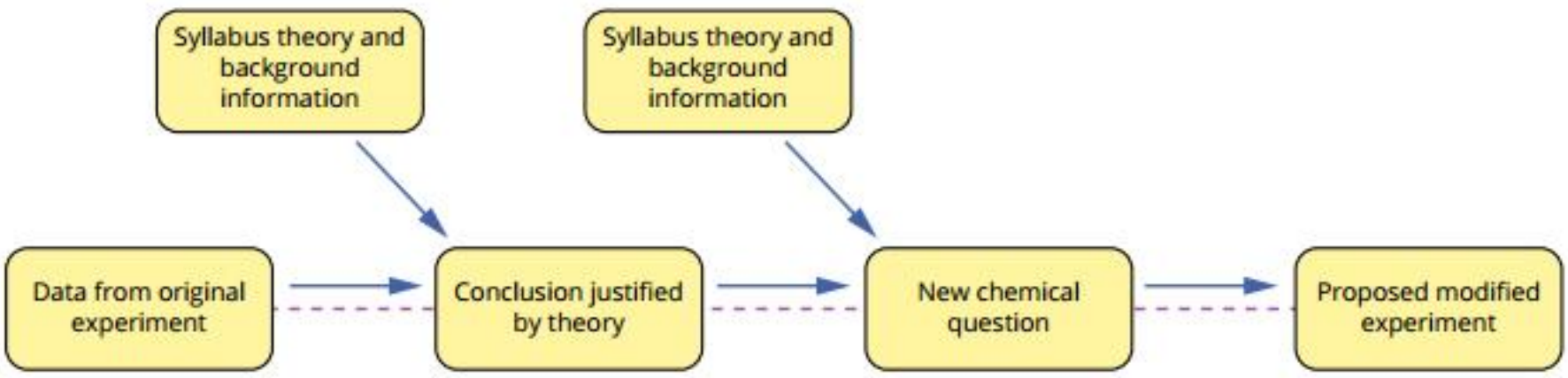

Syllabus theory and background information
Syllabus theory and background information
Data from original experiment
Conclusion justified by theory
New chemical question
Proposed modified experiment

FIGURE 1.9.1 Idea flow for the reasoning process involved for the rationale.

A new chemical question is developed from chemical understanding and the result of the original experiment.

Background information

The chemical concepts of both the original experiment and the proposed new experiment need to be described but it is important to restrict this to the necessary information—a full topic explanation or literature review is not required. Make sure that key syllabus concepts are included using relevant chemical equations, structures and diagrams. Background concepts from scientific literature need to be referenced using in-text referencing. You will need to read widely but limit your use of chemical concepts to the scope of the syllabus. If your original experiment and proposed new experiment cannot be explained using syllabus concepts from the appropriate unit, change your experimental focus. A summative student experiment needs to be based on science understanding from Units 3 and 4. Your explanation of background information demonstrates understanding and knowledge of the direct, and possibly indirect, relationship between the independent and dependent variables and controlled or measured variables.

The syllabus states that the task requires students to 'research relevant background scientific information to inform the modification of the research question and methodology'.

Here we see:

- 'relevant' which means background scientific information related to the syllabus as well as relevant to your experiment
- 'inform' which means you have used science concepts to identify a new experiment
- 'modification' which means the new experiment is related to the first one but the variable(s) and/or method are modified.

Group planning

Parts of the experiment can be completed with your group. For instance, it is appropriate to discuss the findings of the original experiment to be clear about the relationship shown in the data. Also, the group could discuss changes to the method or dependent and independent variables which may be appropriate. You will collect data together; however, the rest of the investigation including analysis, evaluation and report writing is an individual task.

Discuss what you have already learnt in class about the topic and possible or expected relationships which could be investigated (Figure 1.9.2). Develop a specific research question stating the proposed dependent and independent variables. This relationship will be the focus of your research question. In addition, you may propose a refinement of equipment or methodology which will need to be discussed and clarified with your teacher. Check that your school laboratory has the resources for you to perform the experiment or investigate the topic. Choose a topic that can provide clear measurable data that shows how variable y depends on variable x.

Consider the following when developing the modified experiment:

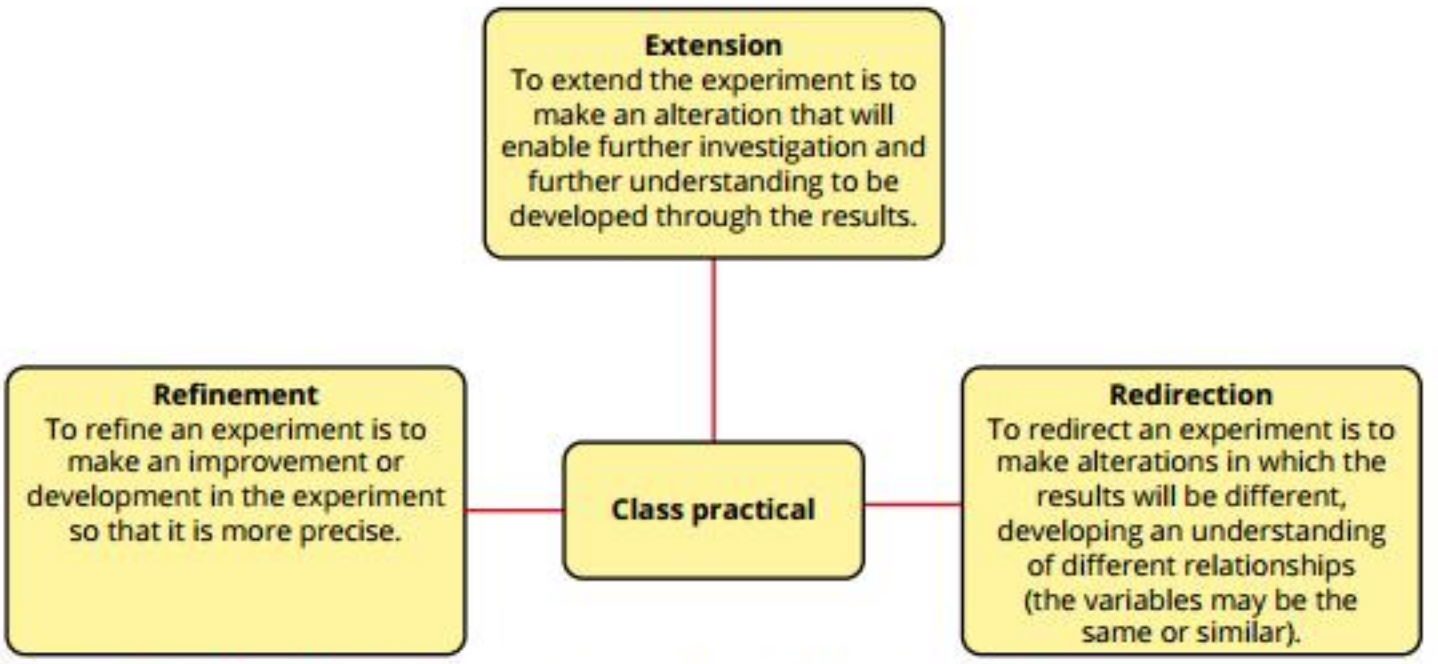

Extension
To extend the experiment is to make an alteration that will enable further investigation and further understanding to be developed through the results.
Refinement
To refine an experiment is to make an improvement or development in the experiment so that it is more precise.
Class practical
Redirection
To redirect an experiment is to make alterations in which the results will be different, developing an understanding of different relationships (the variables may be the same or similar).

FIGURE 1.9.2 Changes that can be made to a practical to develop the student experiment.

Table 1.9.1 shows examples of changing an original experiment into a topic of interest for a student experiment.

TABLE 1.9.1 Examples of modifying a practical into a student experiment

Original experiment	Possible modified experiments
Conduct a calorimetry experiment to measure the enthalpy of the combustion of hexanol.	Does using less water in the calorimeter increase the accuracy in determination of the combustion of hexanol?
	Is the accuracy of the molar heat of combustion of hexanol improved by using multiple trials?
	Can the experimental method be used to determine molar heat of combustion of other alcohols?
	Can the apparatus be altered to limit heat loss and increase accuracy of enthalpy of combustion of hexanol?

Defining the variables and data collection

The factors that can change during your experiment or investigation are called variables. An experiment or investigation determines the relationship between variables by measuring the results. There are four categories of variables (Figure 1.9.3). You should have only one **independent variable**. Otherwise, you could not be sure which independent variable was responsible for changes in the **dependent variable** (the results). It is best to think of a single variable (independent variable) that may influence the measured outcome (dependent variable). Use clear dependent and independent variables, include values for concentrations, and be specific about number of trials. The more variables that are altered (including **measured variables** and **controlled variables**), the more complex the task becomes.

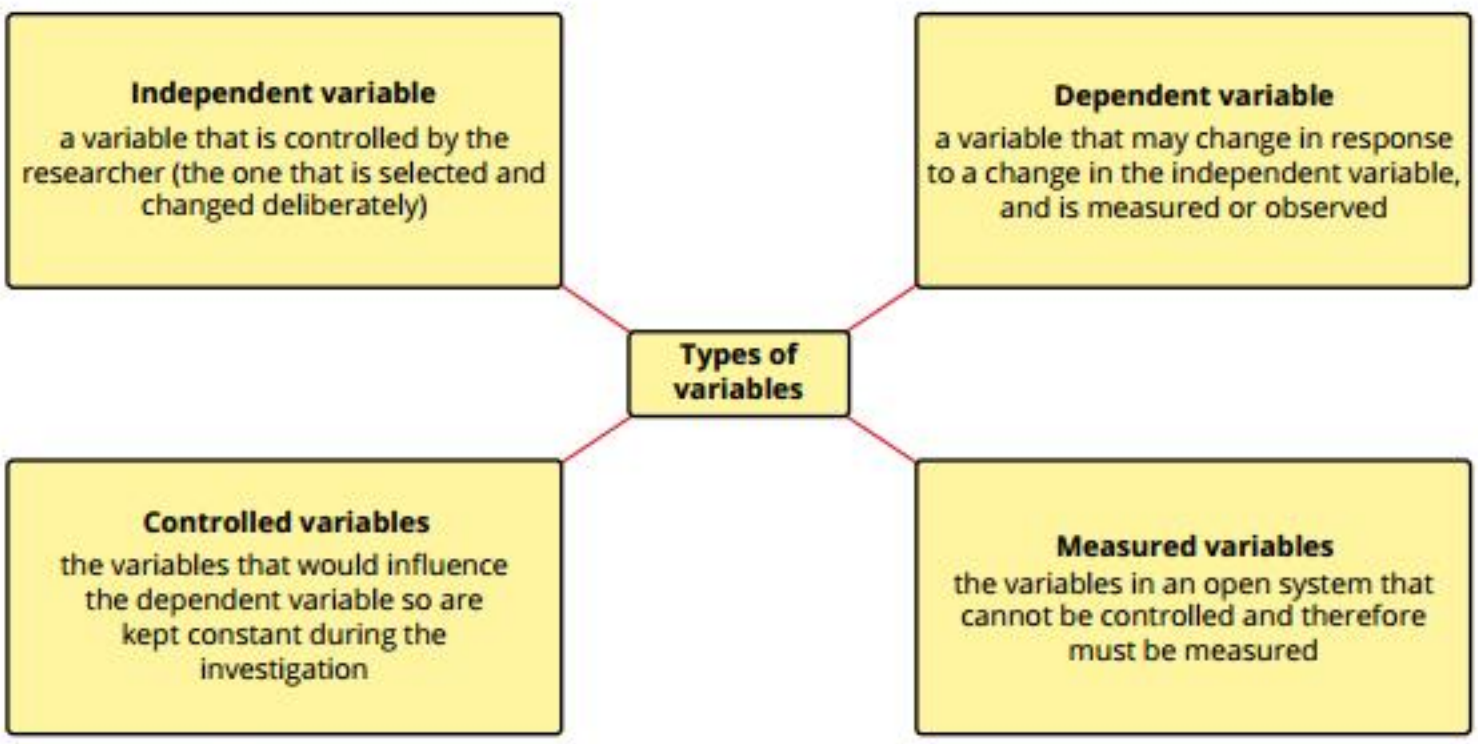

Independent variable
a variable that is controlled by the researcher (the one that is selected and changed deliberately)
Dependent variable
a variable that may change in response to a change in the independent variable, and is measured or observed
Types of variables
Controlled variables
the variables that would influence the dependent variable so are kept constant during the investigation
Measured variables
the variables in an open system that cannot be controlled and therefore must be measured

FIGURE 1.9.3 The four types of variables in experiments.

To ensure an investigation is **valid**, it should be designed so that only one variable is being changed at a time. The remaining variables must remain constant so that meaningful conclusions can be drawn about the relationship between variables. In junior science, we learn "Change one thing, measure one thing, keep everything else the same". In your Rationale and Research Question discussions with your group and teacher, you will consider the:

- independent variable (the thing that is changed)
- dependent (measured) variable
- controlled variables (parts of the equipment, method and conditions that are constant)
- appropriate raw data that will be collected (quantitative versus qualitative), and how each will be measured, collected or controlled.

Data can either be qualitative or quantitative. **Qualitative data** is descriptive and unmeasurable and uses descriptions or adjectives to record observations. It cannot be statistically analysed. **Quantitative data** is empirically measurable and uses instruments to record observations as numbers with units.

Qualitative and quantitative data have further subsets in each category (Figure 1.9.4).

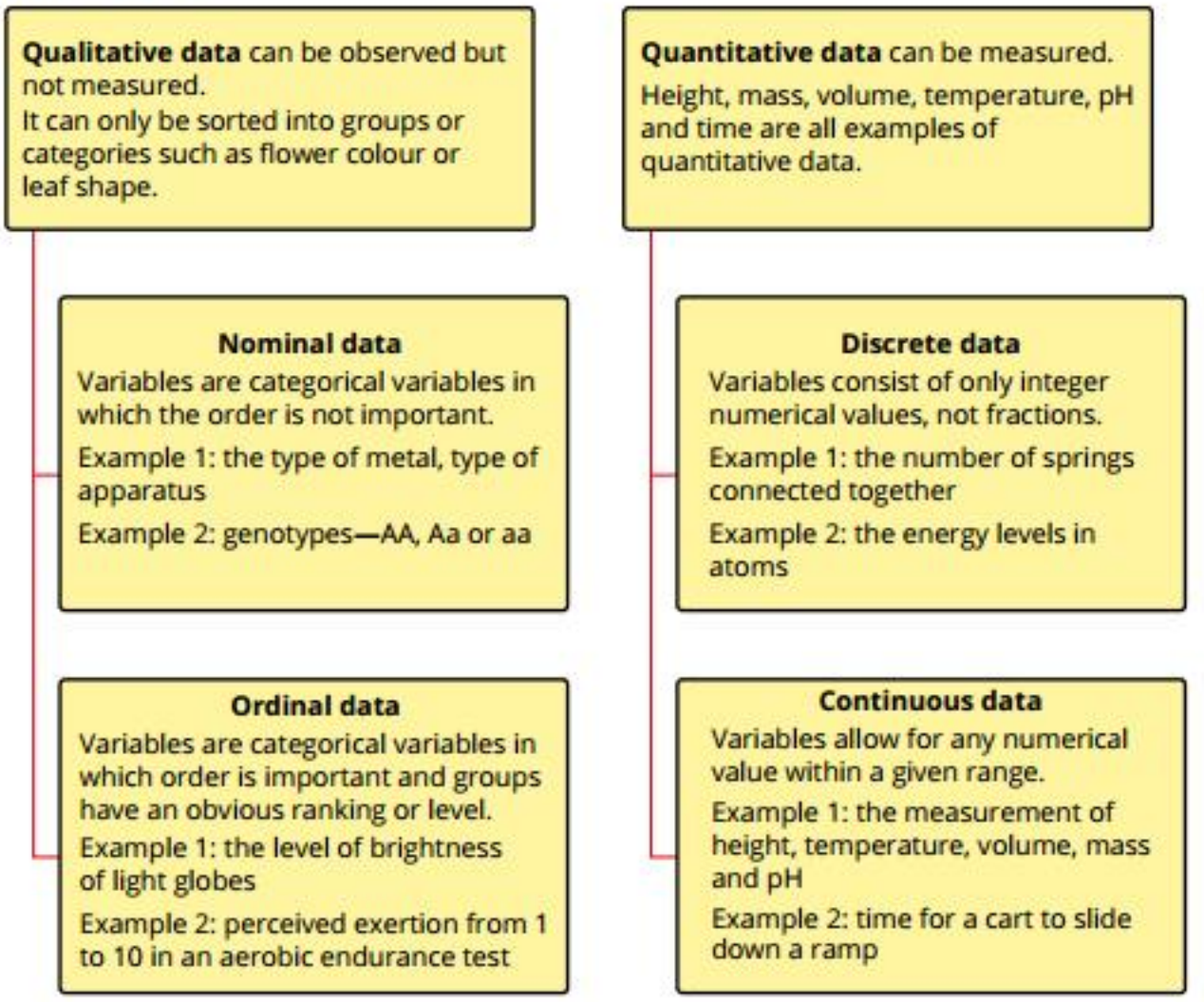

Qualitative data can be observed but not measured.
It can only be sorted into groups or categories such as flower colour or leaf shape.
Quantitative data can be measured.
Height, mass, volume, temperature, pH and time are all examples of quantitative data.
Nominal data
Variables are categorical variables in which the order is not important.
Example 1: the type of metal, type of apparatus
Example 2: genotypes—AA, Aa or aa
Discrete data
Variables consist of only integer numerical values, not fractions.
Example 1: the number of springs connected together
Example 2: the energy levels in atoms
Ordinal data
Variables are categorical variables in which order is important and groups have an obvious ranking or level.
Example 1: the level of brightness of light globes
Example 2: perceived exertion from 1 to 10 in an aerobic endurance test
Continuous data
Variables allow for any numerical value within a given range.
Example 1: the measurement of height, temperature, volume, mass and pH
Example 2: time for a cart to slide down a ramp

FIGURE 1.9.4 Quantitative and qualitative variables.

Measurement of temperature requires an instrument and provides quantitative data whereas sensing the production of heat by touch provides qualitative data (Figure 1.9.5).

FIGURE 1.9.5 (a) A liquid thermometer for measuring water temperature. (b) Feeling heat radiating from a heater is an example of qualitative data as it is based on personal observation. Qualitative data cannot be statistically analysed.

Depending on the experiment, it may be appropriate to record the qualitative observation (e.g. colour change or precipitate formation during a chemical reaction), or perhaps measure the quantitative results (e.g. voltage of a Galvanic cell).

Sourcing appropriate equipment and materials

You will need to decide on the materials, technology and instrumentation that will be used to carry out your experiment or investigation. It is important to find the right balance between items that are easily accessible and those that will obtain accurate and precise results. The precision of the chosen instrumentation affects the level of measurement uncertainty and is recorded as a ± value in the raw data table. Instrumentation choices are described in 'Justified modifications to the methodology'.

Sample size

Because a single measurement or experimental result could be affected by errors, **replication** of samples within an experiment and **repeat trials** are key components of reliability. A larger sample size will improve:

- the representation of the phenomenon
- identification of natural variation, errors and uncertainty
- the results by offering more evidence to support the experimental results
- aids with repeatability and therefore reliability.

Consider the practicalities of timing and validity of data in determining the number of trials and the number of independent variables tested. Given that 10 hours are allocated to planning the experiment, performing the experiment and writing the report, consider that about 15 trials may be sufficient. At least 3 trials per independent variable are generally required. If you are expecting a linear relationship, 3 values of the independent variable may be sufficient but if the expected relationship is logarithmic, 5 or more data points would be required.

This issue is further described in 'Collection of sufficient and relevant raw data' (page e81).

Writing a research question

When you have decided on a dependent variable, independent variable, controlled variable(s) and method of testing, you are ready to write your research question.

A research question directs and describes the scientific inquiry activity. Its purpose is to focus the student experiment, inform the direction of the research and guide all stages of inquiry, analysis, interpretation and evaluation.

The question determines the experiment and the experiment is testing the question. A research question should:

- be specific and relevant to the class experiment
- clearly identify the subject matter of the experiment
- specify the scope or conditions of the inquiry
- aim to find trends or patterns of relationships between two variables.

A research question should state the independent and the dependent variables. It should ask if the independent variable will affect the dependent variable. The research question must specifically outline variables in a way that is measurable; this also allows the research question to be answered.

Look at this example below.

independent variable

'How does changing the concentration of the HCl affect the rate of the reaction between HCl and Mg as shown by reaction time at completion when temperature and mass of Mg are constant?'

dependent variable

A well-constructed research question should have the following characteristics.

- It should include measurable variables—the independent variable and the dependent variable.
- It should have a guiding word, such as *how*, *what* or *will*.
- It should be phrased so that a definitive answer can be developed.
- It should state key (not all) controlled variables or conditions.
- It can state a proposed relationship.

Table 1.9.2 gives examples of constructed research questions.

TABLE 1.9.2 Structuring a research question

Guiding word(s)	Example research questions
will	Will increasing the reaction temperature (10°C, 20°C, 30°C) increase the rate of the reaction between 2 g zinc pieces and 20 mL 0.5 M hydrochloric acid?
how	How does changing the concentration of the cathode solution, $Cu(NO_3)_2$, from 0.1 M to 2.0 M, while keeping the anode, $Zn(NO_3)_2$, concentration constant (0.1 M), affect voltage produced by a Galvanic cell?
can	Can an increase in particle size decrease the rate at which 25 g solid sugar dissolves in 100 mL 20°C water?
do/does	Does acid concentration (0.1 M, 0.3 M, 0.6 M) affect conductivity of H_2SO_4 and HCl solutions at 25°C?

Evaluating your research question

Once a research question has been developed, stop to evaluate it before progressing. Follow the prompts in the chart below (Figure 1.9.6) to refine and improve it.

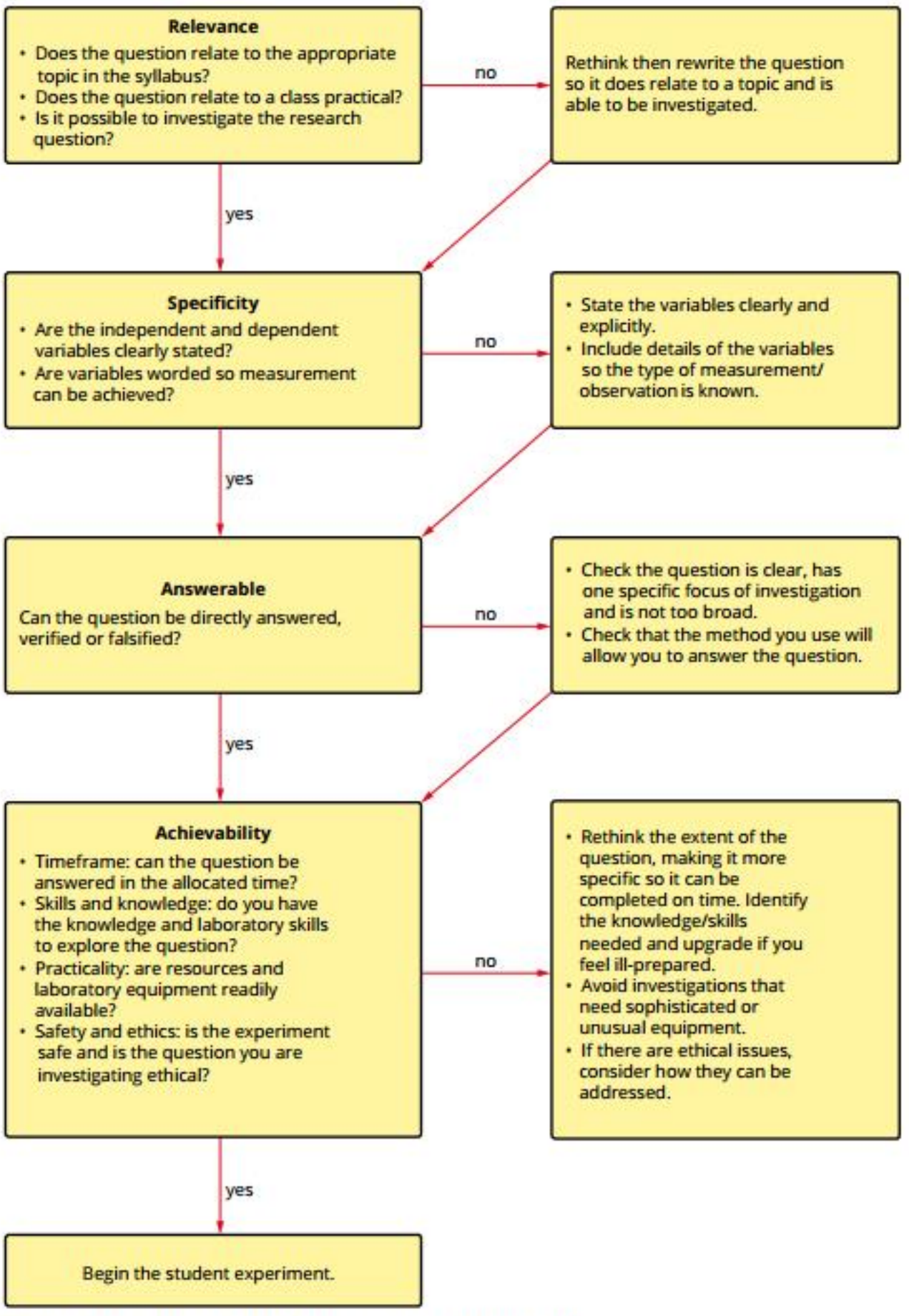

Relevance
• Does the question relate to the appropriate topic in the syllabus?
• Does the question relate to a class practical?
• Is it possible to investigate the research question?
no
Rethink then rewrite the question so it does relate to a topic and is able to be investigated.
yes
Specificity
• Are the independent and dependent variables clearly stated?
• Are variables worded so measurement can be achieved?
no
• State the variables clearly and explicitly.
• Include details of the variables so the type of measurement/ observation is known.
yes
Answerable
Can the question be directly answered, verified or falsified?
no
• Check the question is clear, has one specific focus of investigation and is not too broad.
• Check that the method you use will allow you to answer the question.
yes
Achievability
• Timeframe: can the question be answered in the allocated time?
• Skills and knowledge: do you have the knowledge and laboratory skills to explore the question?
• Practicality: are resources and laboratory equipment readily available?
• Safety and ethics: is the experiment safe and is the question you are investigating ethical?
no
• Rethink the extent of the question, making it more specific so it can be completed on time. Identify the knowledge/skills needed and upgrade if you feel ill-prepared.
• Avoid investigations that need sophisticated or unusual equipment.
• If there are ethical issues, consider how they can be addressed.
yes
Begin the student experiment.

FIGURE 1.9.6 Steps to refine and improve the research question.

A hypothesis is a statement that proposes a relationship between variables and an expected result of the experiment—it is based on some level of understanding. Having completed extensive background research (Rationale), you will have the means and understanding to state the expected results in the form of a hypothesis.

The student experiment does not require a hypothesis and it may not always be appropriate or beneficial. Because the hypothesis proposes a specific relationship between the independent and dependent variables, the hypothesis can either be supported or refuted by the results. Figure 1.9.7 shows key components of a hypothesis.

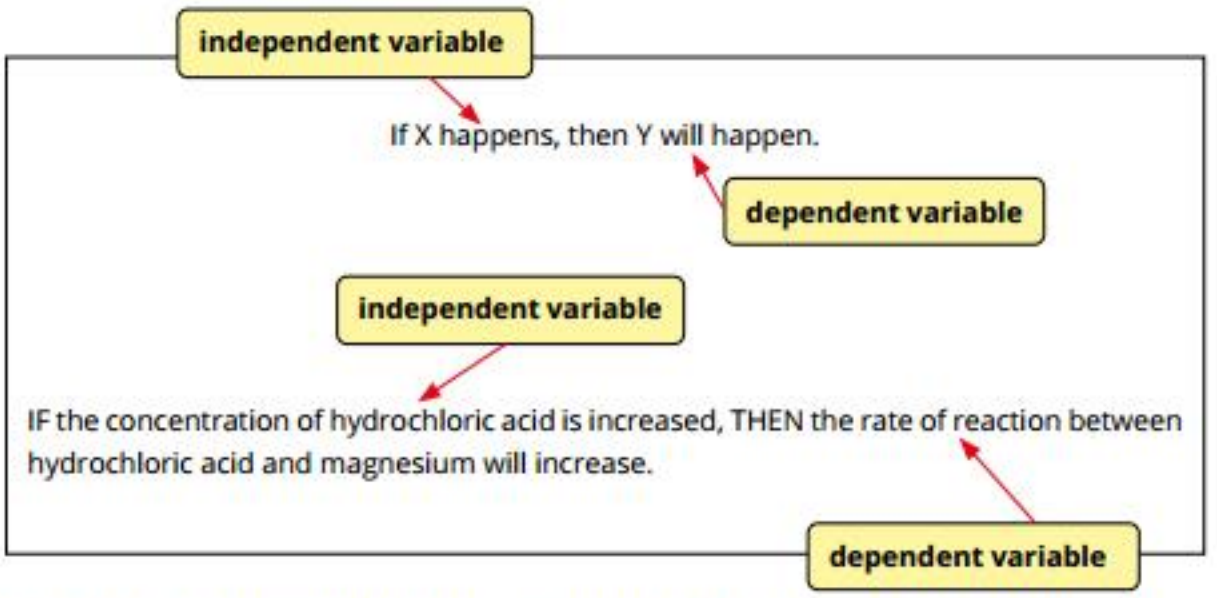

independent variable
If X happens, then Y will happen.
dependent variable
independent variable
IF the concentration of hydrochloric acid is increased, THEN the rate of reaction between hydrochloric acid and magnesium will increase.
dependent variable

FIGURE 1.9.7 The key cognitions in the development of the research question— in terms of the dependent and independent variables.

Table 1.9.3 shows research questions and the associated relationship between the dependent and independent variables.

TABLE 1.9.3 Research question examples

Relationship between dependent and independent variables	Research question
As the temperature of the gas increases, the volume of the gas will increase.	How does the volume of air in a syringe change as the temperature of the air is increased from 20 to 80 degrees Celsius?
The rate of reaction will increase and time for production of 25 mL gas will decrease as the temperature of the reaction mixture increases.	Does the time taken for the production of 25 mL of hydrogen gas decrease as the temperature of the solution of 50 mL 0.5 M hydrochloric acid and 5 g zinc is increased?
The accuracy of the measured molar enthalpy of combustion of ethanol will be increased by performing multiple calorimetry experiments.	Does burning different masses of ethanol (2 g, 4 g, 6 g) in multiple calorimetry experiments improve the accuracy of the determination of the molar heat of combustion?

i A research question proposes a question about the relationship between the dependent and independent variables of the investigation. It is a required component of the student experiment.

A hypothesis defines the expected link between dependent and independent variables and supports the research question but is not an assessed component of the ISMG.

Justified modifications to the methodology

The previous section shows the complexity of the Forming (planning) part of the student experiment. You (and your group and teacher) will have decided on key aspects of the modified experiment—independent, dependent and controlled variables, identified a procedure and equipment for use and written a research question. It is necessary to document each modification to the original experiment in your report and justify each proposed modification.

The methodology of your experiment is a specific step-by-step procedure which your teacher will require you to prepare prior to the experiment. However, this detail is generally not required in the report. In the modifications section, write an overview of the original method (use an in-text reference) in paragraph form and provide a written or tabulated description of the modifications proposed. Include specific details about instruments, chemicals (with concentrations), techniques employed and number of trials. Each modification is justified by stating the type of change ('refine', redirect' or 'extend') and how it will improve the investigation. If possible, link each modification to random and systematic error. An example is shown in Table 1.9.4.

TABLE 1.9.4 Examples of changes to the original experiment with justification

Modification	Type of change	Justification
Replacing the filter paper salt bridge with an agar salt bridge.	Refinement	Provides consistent circuit connection and ion flow and reduces random error.
Collection of more data—five trials for each concentration rather than one.	Refinement	Provides an average and uncertainty of evidence.
Measuring the cell potential difference of one Zn/Zn^{+2} | Cu/Cu^{+2} galvanic cell.	Redirection	Investigates the effect of concentration change on the cell potential of one galvanic cell.
Use a range of concentrations of copper nitrate solutions, consisting of 0.1 M, 0.5 M, 1 M, 1.5 M, 2 M.	Extension	Provides an understanding of how the concentration of a substance can affect the cell potential of the galvanic cell.
Pasco digital bluetooth voltmeter rather than a Dick Smith analog voltmeter.	Refinement	Provides more reliable readings of voltage and reduces possible systematic error.

One way to modify an original experiment is to improve the precision of the laboratory equipment. With higher-precision instruments, there is less chance of error and lower uncertainty in the measurement. Table 1.9.5 demonstrates the benefits of greater-precision instruments through lower measurement uncertainty.

TABLE 1.9.5 The difference in measurement uncertainty between instruments: (a) a glass thermometer with a precision of ±2.5°C; (b) a measuring beaker with a precision of ±5 mL; (c) a digital laser thermometer with a precision of ±0.2°C; and (d) a measuring cylinder with a precision of ±0.25 mL

Lower-precision instruments	Higher-precision instruments
a	c
b	d

PUTTING IT ALL TOGETHER

The sample experiment report shown below is suitable for assessment of Unit 2 and follows the ISMG criteria. While this example may be used as a reference tool, note that IA2 must relate to Unit 3 subject matter.

An investigation into the effect of concentration on the temperature of crystallisation of potassium chloride.

Rationale

Water is an effective solvent because it dissolves polar covalent and ionic substances. Ionic compounds dissolve due to ion–dipole attraction. Oxygen's electronegativity (3.5) and hydrogen's electronegativity (2.2) create a dipole in water, attracting ions. This process is shown in Figure 1 with potassium chloride (KCl). The solubility of a substance is dependent on these interactions occurring but is also affected by the strength of the ionic lattice itself. A stronger lattice causes less dissolving but strong interactions between solute and solvent cause more dissolving. Heating the solvent (water) increases solute dissolving due to the increase in kinetic energy of all particles (solvent and solute) which increases collisions as well as increase the movement of bonded atoms (Holmes et al., 2019).

Cooling a saturated solution leads to precipitation (BBC, 2022). In the original experiment, the relationship between solubility (maximum dissolving solute amount) of KNO_3 and temperature was investigated by cooling a KNO_3 solution of known concentration, observing crystallisation and constructing a solubility curve—it was shown that as temperature increases, solubility increased. At 25°C, maximum dissolving amount of KNO_3 was 32 g per 100 g water, and at 40°C, 60 g was the maximum amount dissolved in 100 g water.

In the modified experiment, the precipitation of the ionic compound potassium chloride (KCl) will be investigated

continued

instead of potassium nitrate (KNO_3). The bonds of KCl form a lattice structure (potassium cations (K^+) and chlorine anions (Cl^-), as seen in Figure 2). The strength of the lattice is based on the electrostatic forces between cations and anions (Ashenhurst, 2021). The current experiment seeks to determine the change to solubility of KCl with temperature by constructing a solubility curve. Also, by investigating the dissolving of an ionic compound that has the same cation as the original experiment but a different anion, the current experiment will show the change to lattice strength with change to anion and/or the change to ion–dipole interactions.

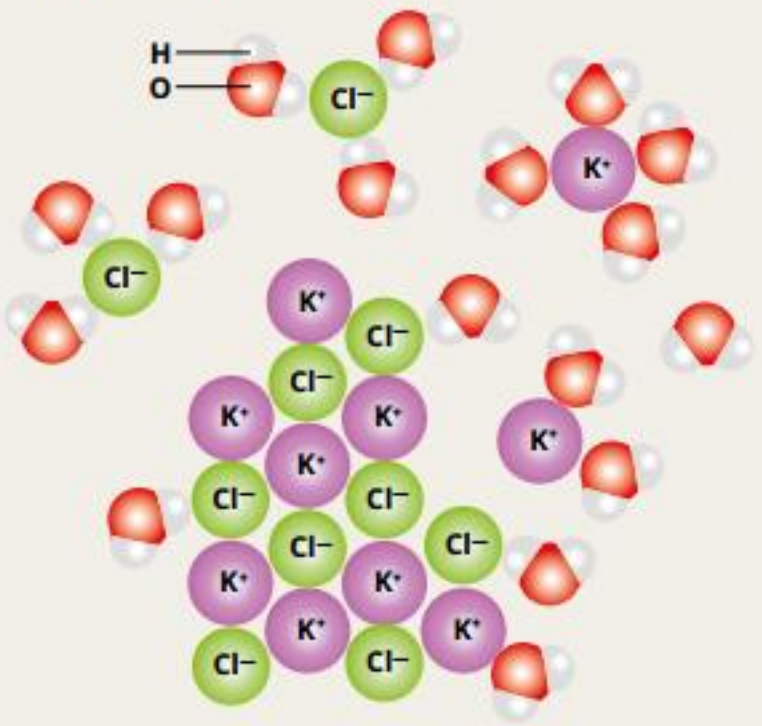


FIGURE 1 H_2O forming dipole interactions with KCl.

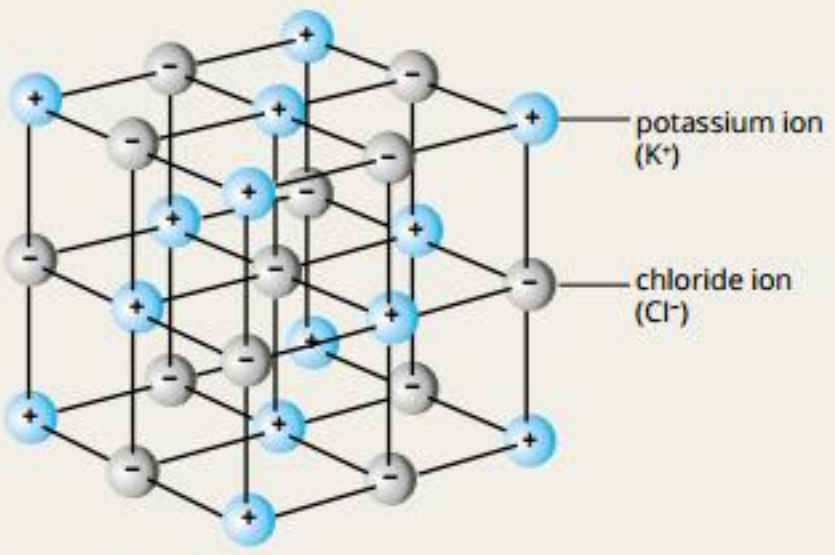


FIGURE 2 Lattice structure of KCl.

Research Question

How does increasing the concentration of KCl (36 g/100 mL, 40 g/100 mL, 44 g/100 mL and 48 g/100 mL) affect the temperature at which crystallisation occurs in a 5 mL solution?

Original Experiment

The initial experiment dissolved the ionic substance, KNO_3, in water at concentrations between 40 g/100 ml and 120 g/100 mL by heating with a Bunsen burner. After dissolution, the test tubes were allowed to cool until crystallization occurred, and the solution's temperature was recorded (Figure 3). The modifications made to this experiment are shown in Table 1.

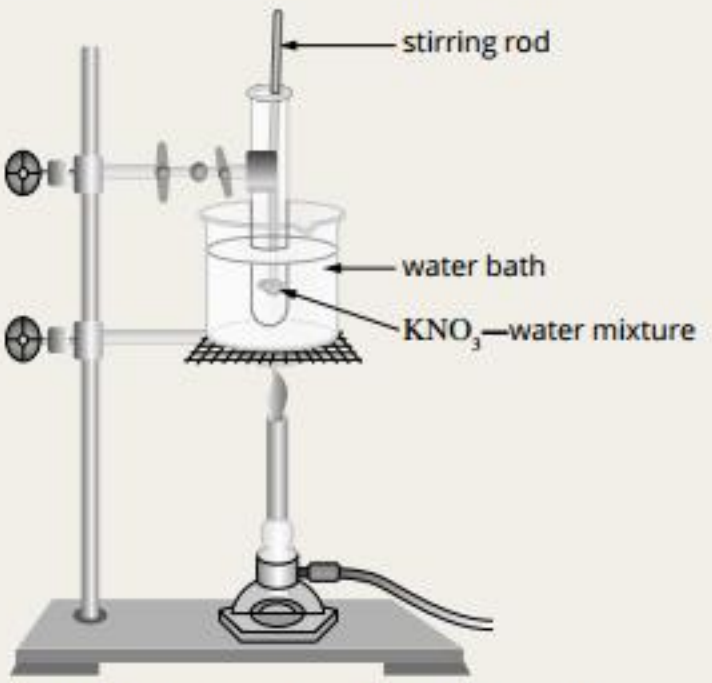


FIGURE 3 Original experiment set-up (Huddart, 2019).

TABLE 1 Modifications to the original methodology

Modification	Justification
The experiment was **refined** by increasing the sample size from one trial to five.	This enables the collection of sufficient raw data so that an average temperature is calculated. Conducting more trials enhances experiment accuracy and reliability by identifying and eliminating anomalies, and identifying the trend.
The ionic compound was **changed** from potassium nitrate to potassium chloride.	Changing the solute allows for a greater understanding of solubility trends of potassium-based ionic compounds.
The Bunsen burner with beaker of water was **refined** to a water bath heated by a hot plate.	Using a heated water bath rather than a Bunsen burner allows for greater accuracy as the temperature stays consistent and is controlled.
An additional concentration was added which **refines** the experiment. 36 g/100 mL, 40 g/100 mL, 44 g/100 mL and 48 g/100 mL	Testing four concentrations instead of three allows for greater confidence in the observed trend.
Expected values are obtained from research and compared to experimental data.	By comparing to expected values, the accuracy and validity of the experiment can be assessed.

FIGURE 4 Experimental set-up—electronic balance, electronic water bath, test tube, rack and funnel, spatula, KCl powder, thermometer.

1.10 Finding

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- conduct a risk assessment
- undertake an experiment encompassing sufficient and relevant data
- collect and present data

RISK ASSESSMENT

When planning for an experiment, it is important for your safety and the safety of others that you consider the potential risks. Risks are potential negative outcomes from carrying out an activity. Everything we do has some risk involved. **Risk assessments** are performed to identify, assess and control risks. A risk assessment should be performed for any situation, whether in the laboratory or out in the field, that could cause harm to people or animals.

The first step in the risk assessment process is to assess all risks in the environment in which the experiment or fieldwork will be carried out. This is the inherent risk. The second step is to identify control measures that will reduce the level of risk to low risk. For example, glass equipment in the laboratory is a hazard as it can cause injury if it breaks. Injury is a negative outcome and so it is a risk. A control measure to reduce this risk is handling the glass equipment carefully.

Your report should outline risks, include values, including detail such as the chemical names and concentration values, and how the risks will be accounted for (managed). While the key consideration is for the personal safety of the people in the laboratory, you need to consider and include a statement about potential effects on the environment. The ethics of the investigation are also considered and managed. Ethical and environmental considerations must be mentioned even if there is no risk.

Your risk assessment will have three sections:

- hazard—the name of the item or activity that could cause risk
- risk—the possible negative outcome that could occur
- control measures—the practices or processes to avoid the risk.

Often, the original experiment will have used similar equipment and so information from its risk assessment can be used. Check with your teacher regarding new equipment that you are planning to use.

To identify risks, think about the following:

- laboratory rules of the school. For example, procedures for correct behaviour in a laboratory and procedures for equipment use
- the activity that you will be carrying out including physical issues such as lifting heavy objects and how you will use any equipment (such as glassware) or chemicals that you will be handling, including sources of heat and electricity
- the facilities of the laboratory. These include emergency equipment on site, ventilation of the laboratory, facilities such as a fume hood
- the chemical codes and SDS (Safety Data Sheet) for chemicals in use. Consider also concentrations of chemicals and hazards associated with products of chemical reactions
- what protective clothing you should wear, e.g. lab coat and goggles.

Chemical codes

The chemicals in the school laboratory or in a hardware shop have a warning symbol on the label. These symbols are a chemical code indicating the nature of the contents (Table 1.10.1). In 2017, the Globally Harmonised System of Classification and Labelling of Chemicals (GHS) was introduced in Australia for use in workplaces, including school laboratories.

TABLE 1.10.1 GHS pictograms used as warning symbols on chemical labels

GHS pictogram	Use	GHS pictogram	Use	GHS pictogram	Use
	flammable liquids, solids and gases; including self-heating and self-igniting substances		oxidising liquids, solids and gases, may cause or intensify fire		explosion, blast or projection hazard
	corrosive chemicals; may cause severe skin and eye damage and may be corrosive to metals		gases under pressure		fatal or toxic if swallowed, inhaled or in contact with skin
	low level toxicity; this includes respiratory, skin and eye irritation, skin sensitisers and chemicals harmful if swallowed, inhaled or in contact with skin		hazardous to aquatic life and the environment		chronic health hazards; this includes aspiratory and respiratory hazards, carcinogenicity, mutagenicity and reproductive toxicity

Safety Data Sheets

Each chemical substance has an accompanying document called a **Safety Data Sheet (SDS)** (Figure 1.10.1). An SDS contains important safety and first aid information about each chemical you commonly use in the laboratory. The SDS provides employers, workers and health and safety representatives with the necessary information to safely manage the risk of hazardous substance exposure.

1. IDENTIFICATION OF THE MATERIAL AND SUPPLIER

Product identifier

Product Name HYDROCHLORIC ACID - 20% OR GREATER

Supplier
Edwards & Tubbs Operations Pty Ltd
ABN: 51 444 444 444
13 Royston Vasey Street
Melbourne 3000
Australia

Emergency telephone number **1900 654 321 (ALL HOURS)**

2. HAZARDS IDENTIFICATION

GHS Classification

Classified as dangerous goods in accordance with the Australian Code for the Transport of Dangerous Goods by Road and Rail (ADG).

Classified as a hazardous chemical in accordance with the criteria of Safe Work Australia - Globally Harmonized System (GHS).

Corrosive to metals	Category 1
Skin corrosion/irritation	Category 1 Sub-category B
Serious eye damage/eye irritation	Category 1
Specific target organ toxicity (single exposure)	Category 3

SIGNAL WORD: Danger

Hazard statements
H290 - May be corrosive to metals
H314 - Causes severe skin burns and eye damage
H335 - May cause respiratory irritation

Precautionary Statements - Prevention
Keep only in original container
Do not breathe fume, gas, mist, vapours, spray
Wash face, hands and any exposed skin thoroughly after handling
Use only outdoors or in a well-ventilated area
Wear protective gloves / protective clothing / eye protection / face protection

FIGURE 1.10.1 Extracts of a Safety Data Sheet (SDS) for concentrated hydrochloric acid. The SDS alerts the reader to any potential hazards when using a substance, including appropriate measures to reduce risk of harm.

All schools store SDS and chemical code information for materials in use in laboratories and these must be consulted when planning investigations. Online platforms such as RiskAssess allow quick access to these data bases for a planned experiment. In these types of software programs, the potential hazards for each aspect of the experiment are provided when proposed equipment and materials are listed. Handling procedures are also suggested.

It is important to note that to address the syllabus requirement to show 'considered management of risk', you need to do more than download a data sheet or risk assessment. The syllabus specification requires you to 'conduct a risk assessment and account for risks in the methodology.' This means that, as described above, the three factors of (i) risk (ii) possible negative outcome and (iii) prevention need to be aligned and clearly presented in the report. This can be done by writing a paragraph or preparing a table (Table 1.10.2). The supporting data sheets or risk assessment should be placed in the Appendix and key facts used in your report.

TABLE 1.10.2 Sample risk assessment table showing hazards, risks and control measures to reduce the risks

Risk assessment		
Hazard	**Risk**	**Control measures**
Glass equipment	Breakage of glass	Cautiously handle Stay aware of surroundings Listen to teachers' commands
1 M copper sulfate	Skin irritation	Gloves
1 M potassium nitrate	Eye irritation	Goggles
1 M zinc nitrate	Inhalation: light headedness, respiratory irritation	Face mask Handle powder gently
Zinc metal	Cuts	Cautiously handle
Copper metal	Skin irritation	Gloves

Risk controls

The hierarchy of risk controls is shown in Figure 1.10.2. It is organised from the most effective to least effective. The most commonly used risk control measure that addresses the majority of risks is personal protective equipment. The least common but most protective control measure is eliminating the risk from the scientific investigation.

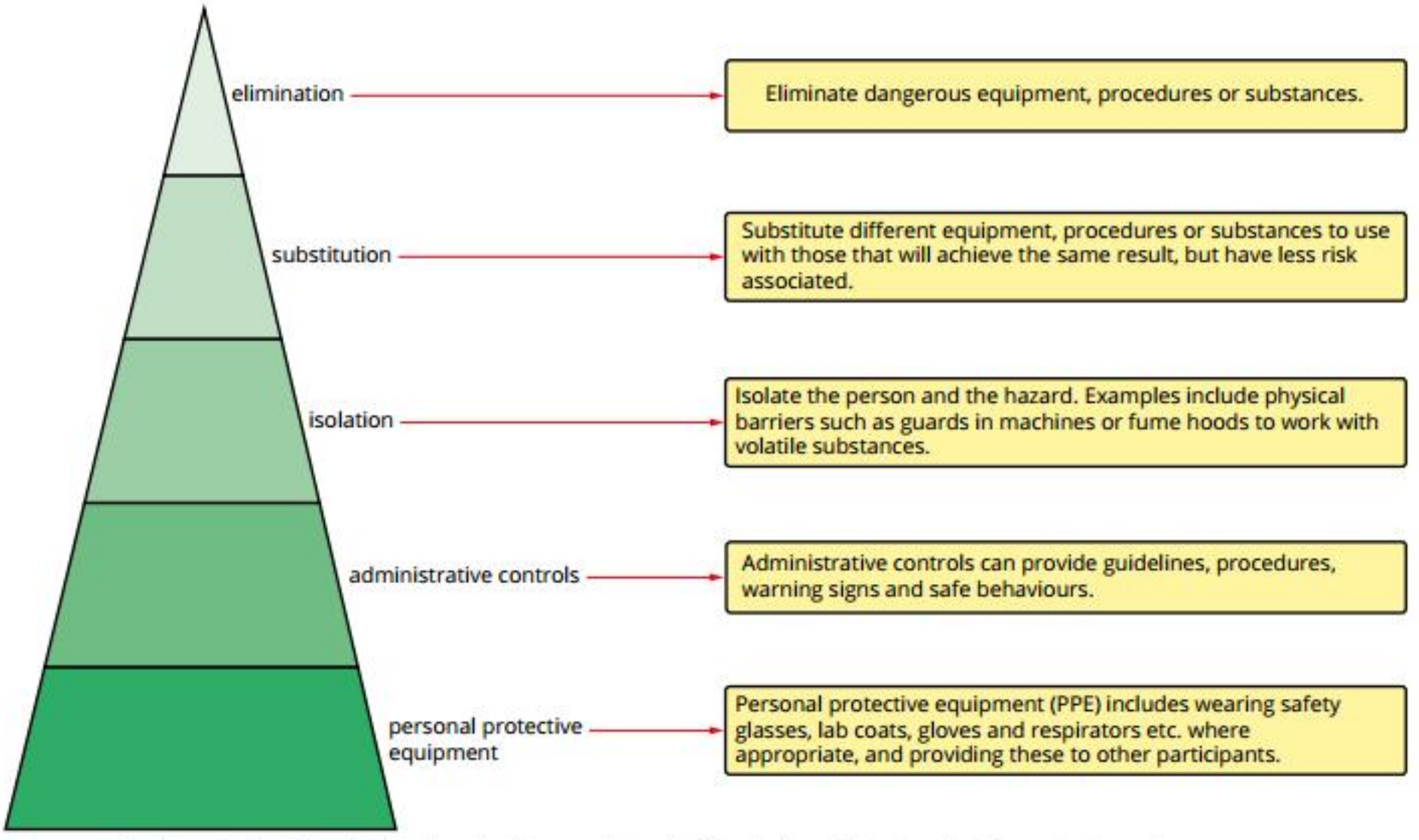

elimination
Eliminate dangerous equipment, procedures or substances.
substitution
Substitute different equipment, procedures or substances to use with those that will achieve the same result, but have less risk associated.
isolation
Isolate the person and the hazard. Examples include physical barriers such as guards in machines or fume hoods to work with volatile substances.
administrative controls
Administrative controls can provide guidelines, procedures, warning signs and safe behaviours.
personal protective equipment
Personal protective equipment (PPE) includes wearing safety glasses, lab coats, gloves and respirators etc. where appropriate, and providing these to other participants.

FIGURE 1.10.2 The hierarchy for risk control is shown in this pyramid, marked from bottom to top in order of increasing importance.

Personal protective equipment

Everyone who works in a laboratory wears items that help keep them safe, such as those shown in Figure 1.10.3. These items are called **personal protective equipment (PPE)** and include:

- safety glasses
- shoes with covered tops
- disposable gloves when handling certain chemicals
- a disposable apron or a lab coat if there is risk of damage to clothing
- hair net or tied back hair for using a Bunsen burner.

FIGURE 1.10.3 Examples of PPE shown are protective eye wear, lab coats and gloves.

Environmental and ethical considerations

When planning an investigation, identify all possible environmental and ethical considerations and evaluate mitigation of issues. Reactants and products of chemical reactions are often toxic to aquatic organisms and, because our wastewater will eventually re-enter the natural environment, many common laboratory solutions (for example, metal sulfates and metal nitrates) must be collected for special disposal rather tipped in a sink.

Ethics is a set of moral principles by which your actions can be judged as right or wrong. Scientists have to obtain approval from an ethics committee and follow ethical guidelines relating to animals and humans. In reality, school chemistry investigations generally have minor ethical issues, if any. However, consider if during the experiment, one party or group benefits over another, or are there real-world connotations of the investigation not accepting of the rights of a community group.

COLLECTION OF SUFFICIENT AND RELEVANT RAW DATA

Enough data needs to be collected to substantiate whether or not a relationship exists between the dependent and independent variables. For the data to be relevant, the investigation must collect values for independent and dependent variables as described in the Research Question. For the data to be *sufficient* means to have appropriate sample size in terms of an appropriate number of replicate trials and an appropriate number of variations of the independent variable. Sample size will affect the accuracy of the data, the uncertainty within the data collected and the ability to interpret the data. In general, a minimum of five data points and three measurements per data point (three trials), or three data points with five measurements per data point (five trials) are needed. This provides a sample size consistent with sufficient and relevant data. Consider your expected trend. If you are expecting a logarithmic or other non-linear trend, you will need at least four or five data points—three would not clearly show the trend. Table 1.10.3 below outlines examples of sample size and their effect on the results of an experiment.

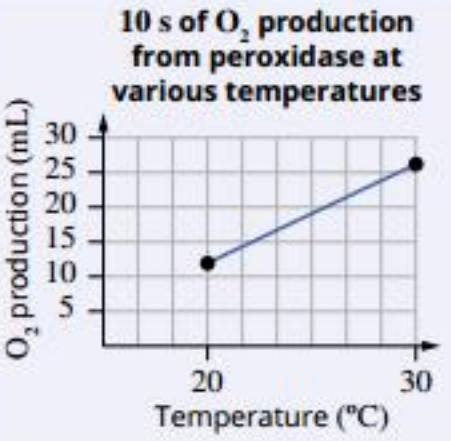
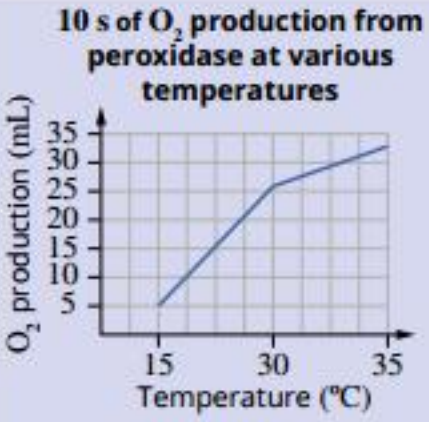
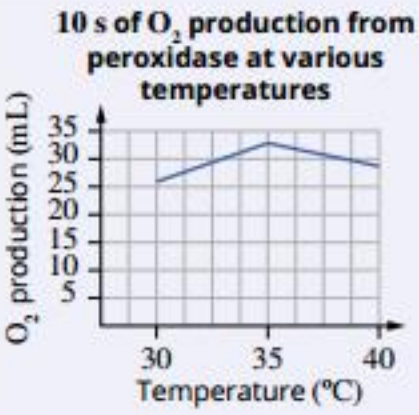
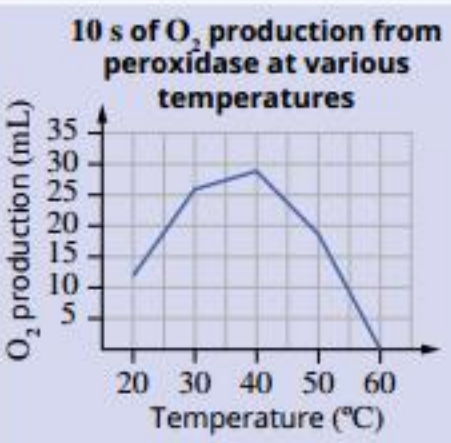
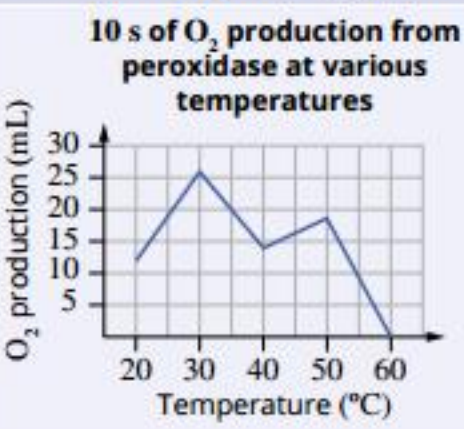
Having determined your sample size, check with your teacher that your protocol and schedule (methodology) are appropriate. You need to be able to perform your experiment independently, in the time available in the school laboratory, and with minimal support from your teachers and school laboratory staff.

It is common for experimentation and testing not to go according to plan even if comprehensive background research has been undertaken. Refinements such as reducing or increasing the sample size may be necessary due to timing issues, change to instrumentation or resource limitation.

If the expected data is not obtained, do not worry. Sometimes a different point of view, such as from a fellow student or a teacher, is all that is needed to find a solution. As long as the data can be critically and objectively evaluated (limitations of the investigation are identified) in your report, the work is worthwhile. Unexpected data provides students with an opportunity to add depth to their experimental report by critically evaluating issues in the experiment. There may be evidence of extraneous variables (not previously recognised) or confounding factors. Evaluation of the methodology based on evidence collected and suggested improvement(s) is a key section of the scientific report. This is discussed further in Module 1.12.

Record everything. Your data set may contain both quantitative (values and measurements) and quantitative (observations) data. Note any difficulties encountered or trials which were conducted slightly differently—perhaps a new source of a chemical was provided half-way through, a new measuring instrument, or a different person determining the readings. This information may be key to your analysis and evaluation. With justification, a data point can be identified as an **anomaly** and removed from the data set due to being an outlier. This may be due to a mistake or failure to correctly follow the method (see 'Processing the data' on page e86). Nevertheless, all values need to be recorded in the raw data table. Choosing not to record certain measurements or observations is invalid, shows bias

TABLE 1.10.3 Examples of sample size and their effect on an experiment

Example of analysed data	Effect of sample size on analysis
	A line graph with two sample points: With only two individual sample points, these results suggest an inappropriate relationship between temperature and enzyme activity; that enzyme activity increases with temperature.
	Line graph with three sample points using an uneven scale: The spread between the chosen individual sample points is inappropriate for this experiment as they should be evenly spread. This example produces results with an incorrect relationship between temperature and enzyme activity; that enzyme activity increases then begins to level off as temperature increases.
	Line graph showing limited sample points: The chosen number of individual sample points is appropriate. This may be sufficient; however, the next example provides more precision and validity for the relationship.
	Scatterplot with appropriate number and distribution of sample points: The number of individual sample points here best demonstrates the relationship between the variables.
	Line graph based on data that had no replicates (only one trial): These results are due to only a single trial for each individual sample point (distance) without any replicates. In this example, the measurement at 40°C was a mistake, and without replicates these mistakes will influence the results.

and is scientifically fraudulent. Quality scientific analysis processes the raw data as it is and is open to any result. Module 1.11 describes how precision and validity can be assessed using calculations such as the percentage error, the percentage uncertainty and the uncertainty of the mean.

A workable plan for data collection is for one group member to be responsible for recording. This minimises clutter at the experimental work bench and provides a consistent single data set to share with the group. The recording person should add the measurement uncertainty of each piece of equipment or instrument as a range of data next to the measured value (e.g. measurement ± Δ measurement). Conducting the experiment and collecting data is a group activity; however, all subsequent parts of the task (data processing, analysis, evaluating and concluding) are completed individually. Therefore, it is important that the data set is disseminated to the group immediately after the experiment finishes.

Electronic data acquisition in schools

Electronic data acquisition takes advantage of highly accurate sensors to collect data directly for processing by a computing device (Figure 1.10.4). There are many sensors, probes and instruments available that can measure a vast variety of phenomena in a single device.

FIGURE 1.10.4 Data acquisition software produces real-time graphs that can be downloaded or printed.

Many smartwatches (Figure 1.10.5) and apps in phones include digital sensors and **data loggers** that can be accessed and used for some class practicals and experiments.

Recording is done accurately and can be continuous or manual, and the measurements are saved electronically. The saved measurements can then be accessed via a computer or directly from the tablet screen. The rate at which measurements are recorded is called the sample rate. Data capture rate can be varied from 100 000 times per second through to once an hour.

FIGURE 1.10.5 Many smartwatches and phones have digital sensors and in-built data loggers.

PUTTING IT ALL TOGETHER

The sample experiment report that follows covers the ISMG criteria. Use this as a model for reference.

Management of Risks

Potassium chloride solution at this concentration (48 g/100 g, 6.4 mol L^{-1}) poses no significant risk, but eyewear should still be used to prevent eye contact with the powder (Risk Assess, 2022).

Handling glassware and a glass thermometer carries inherent hazards and may lead to personal injury. Thus, it's crucial to handle equipment with care, and any breakage should prompt immediate notification of a teacher.

Additionally, solutions should be placed at the centre of the table to minimise the risk of breakage.

Using a hot plate to heat the water bath poses a risk of electrocution. To mitigate this, spillages should be avoided, and the water bath should be positioned centrally on the hot plate. In case of spillage, immediate alerting of a teacher is necessary.

There are no ethical or environmental risks.

Results—Raw Data

TABLE 2 Temperature at which KCl precipitated (raw data)

		Temperature Precipitation Occurs (±0.5°C)				
		Trials				
Concentration of KCl (g/100 ml)	**Concentration of KCl (g/5 ml)**	**1**	**2**	**3**	**4**	**5**
36	1.8	28*	35.5	37	36.5	38
40	2	49.5	48	51.5	52	48.5
44	2.2	67.5	65	64.5	64.5	64
48	2.4	77	75.5	78	74.5	77.5

*significantly different trial; was removed from all calculations

1.11 Analysing

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- process data using a range of mathematical calculations
- present sample calculations
- analyse data to prepare graph(s) and identify trends
- analyse data to identify precision of evidence (using uncertainty) and accuracy of evidence (using % error)

PROCESSING THE DATA (SAMPLE CALCULATIONS)

Processing the data in numerous ways (including mathematical techniques and graphing) allows elucidation of relationships between variables. You will analyse trends or patterns in the data, uncertainties and limitations, outliers and results of significance. To prepare your **processed data**, you should consider which of the following mathematical techniques are suitable in your investigation:

- Mean
- Gradient analysis
- Scatterplot (with best-fit lines, maximum and minimum trendlines and R^2)
- Measurement uncertainty (absolute measurement uncertainty and percentage measurement uncertainty)
- Propagation of measurement uncertainty (addition, subtraction, multiplication, division)
- Uncertainty of the mean (absolute and percentage) formula $\Delta\bar{x} = \pm \frac{(x\text{max} + x\text{min})}{2}$
- Formula: percentage uncertainty (%) $= \frac{\text{absolute uncertainty}}{\text{measurement}} \times \frac{100}{1}$
- Formula: percentage error (%) $= \left|\frac{\text{measured value} - \text{true value}}{\text{true value}}\right| \times \frac{100}{1}$

These seven calculations are explained in Part A: Working scientifically and in the Science Inquiry section of the syllabus.

When you have decided which of these seven calculations are valid for your investigation, prepare a processed data table and include a sample calculation table which shows a single calculation for each. Remember, there are two types of uncertainty—one associated with the measuring equipment (measurement uncertainty) and one associated with the range of trials (uncertainty of the mean). Both of these values can be expressed in the same units as the value they describe (absolute uncertainty) or converted to a percent of the measurement or mean that they describe (percentage uncertainty). See Table 1.11.1.

TABLE 1.11.1 Example of processed data in a table

$CuSO_4$ conc. (M)	Mean cell potential (V)	Absolute measurement uncertainty (V)	Percentage measurement uncertainty (%)	Theoretical E_{Cell} (V)	Absolute error (E)	Percentage error (%)
0.01	1.060	±0	±0	1.040	±0.019	±1.835
0.10	1.073	±0.005	±0.465	1.070	±0.003	±0.269
0.25	1.076	±0.005	±0.464	1.082	±0.005	±0.512
0.50	1.083	±0.005	±0.462	1.091	±0.007	±0.711
1.00	1.086	±0.005	±0.460	1.100	±0.013	±1.212

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When calculations are performed with data values, the uncertainties associated with these values are combined in a process called propagating uncertainties. For example, if a density value is calculated using measured mass and volume, using the relationship density $= \frac{\text{mass}}{\text{volume}}$, then the percentage uncertainty for the measurement of mass (weighing balance) is added to the percentage uncertainty for the measurement of volume (measuring cylinder). This total gives the percentage uncertainty for the density (refer to Part A).

IDENTIFICATION OF TRENDS, PATTERNS AND RELATIONSHIPS

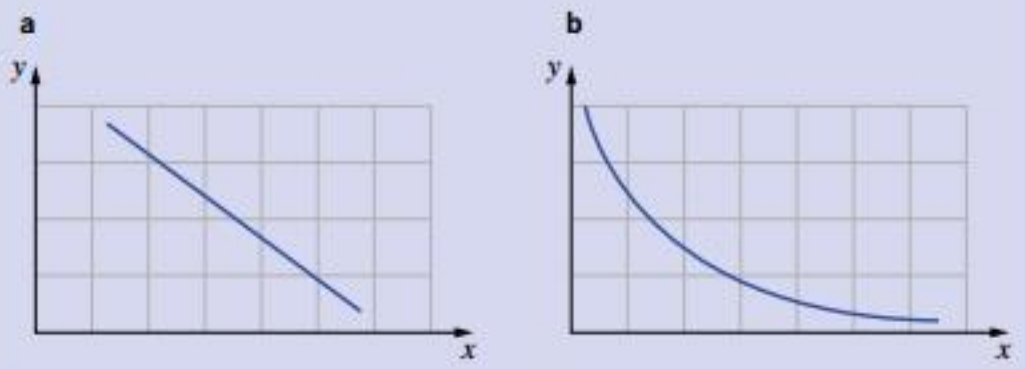
There are a number of ways of presenting processed data, depending on its nature, including tables, graphs, flow charts and diagrams. Usually, a graph is most useful—a clear visual representation showing a direct or inverse relationship between the dependent variable and the independent variable and if the relationship is linear or not. The Excel program will provide information about the trendline gradient and an R^2 value. By plotting expected values (if known) on the same graph, the accuracy of the data is visualised. A number of trends are shown in Table 1.11.2

TABLE 1.11.2 Graphs showing different trends and relationships between variables

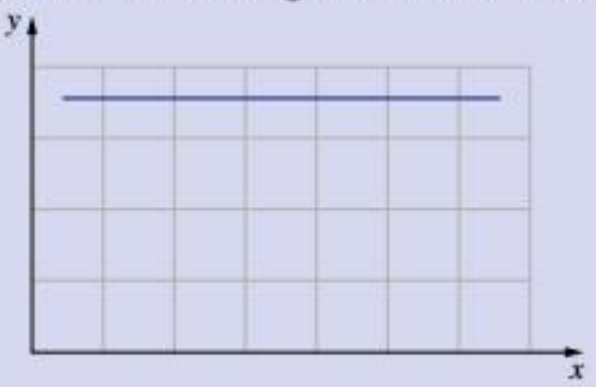
Variables that change in linear or direct proportion to each other produce a straight, sloping trend line.

Variables that change exponentially in proportion to each other produce a curved trend line.

When there is an inverse relationship, one variable increases as the other variable decreases. It may be (a) direct or (b) non-linear.



When there is no relationship between two variables, one variable will not change even if the other changes.



Plotting error bars or maximum and minimum trendlines on a graph indicates if the averages shown are significantly different. Overlapping error bars indicate that the difference between these two values is not statistically significant. The graph(s) that you have prepared provides evidence of the relationship between the dependent and independent variables; however, you should describe the features of the graph using a succinct statement such as 'as (independent variable) increases, (dependent variable) increases/decreases'.

It would be useful to follow this with some values from the graph to justify the occurrence of the trend. Further useful analysis could describe the gradient, R^2 value, similarity/difference to the expected values and whether the error bars overlap or not. Remember, the report has an evaluation section so at this stage it is not necessary to fully explain every aspect of the data. A 'thorough and appropriate identification of trend/patterns/relationships' is what is required here in the Analysis section.

IDENTIFY UNCERTAINTY AND LIMITATIONS OF THE EVIDENCE

Uncertainty, precision and reliability

In chemistry, there is always variation in measurements (the terms precision and uncertainty were explained in Part A). The level of uncertainty is indicated by:

- using values for the measurement uncertainty of the instrument(s) or
- using the range of trials and dividing by 2 (uncertainty of the mean).

Both of these can be expressed as percentage of the value they describe, and both of these give us an indication of the level of random error in the experiment. When identifying and discussing the level of random error, it is most useful to calculate both of these and relate the discussion to the higher value, keeping in mind that, generally, a percentage uncertainty of 5% is the maximum value for a precise and reliable dataset.

Consider these two uncertainty types in an example dataset (Table 1.11.3) which shows the volume of 1.0 M hydrochloric acid required to neutralise 25 mL of an unknown concentration of sodium hydroxide solution. First, the uncertainty due to the precision of the burette (measurement uncertainty) is the smallest increment of the scale, so ± 0.1 mL. When expressed as a percentage of the mean, this is 0.48%.

Second, the uncertainty of the mean is calculated using uncertainty of mean = $\frac{\text{range}}{2}$ giving an uncertainty of ± 0.4 mL. When expressed as a percentage of the mean, this is 1.95%. We see that the uncertainty of the mean is greater than the measurement uncertainty and so we can deduce that the precision of the measurement instrument is only slightly contributing to the level of random error in the experiment. There are further factors contributing to the 1.95% uncertainty.

In addition, as the 1.95% relative uncertainty of the mean is well below 5%, we can state that the data is precise and reliable and that the level of random error in the experiment is low.

TABLE 1.11.3 Volume of 1.0 M hydrochloric acid required to neutralise 25 mL of an unknown concentration of sodium hydroxide solution

Trial	Volume of hydrochloric acid used (mL)
titration 1	20.6 ± 0.1
titration 2	20.9 ± 0.1
titration 3	20.1 ± 0.1
titration 4	20.4 ± 0.1
Mean	20.5 ± 0.4

Percentage error, accuracy and limitations of the evidence

The rationale has provided background information that informs the relationship proposed in the research question. This provides your expected trend, and in your Analysis you will state if this trend was obtained. In addition, you may be able to research expected values for the data set that you have collected. If this is the case, it is expected that you will calculate percentage error values for each independent variable data point.

Percentage error measures how different your data is to expected values and so will allow you to make a judgement about accuracy and validity. Low percentage error indicates low systematic error in the investigation. By researching expected values, you are accessing experimental data from scientific laboratories and so we expect that the equipment and methodology in a secondary school laboratory is unlikely to accurately replicate these values. For this reason, you cannot use '5%' as a guide for acceptable data (as for uncertainty and precision). Percentage error is likely to be higher than this. Nevertheless, if a percentage error value is as high as 50%, you can identify a lack of accuracy and the investigation is lacking validity—state this as a limitation.

Again, when identifying these issues as part of trends, patterns and relationships, resist the temptation to explain and suggest reasons for these results because this discussion is more relevant to the concluding and evaluation sections.

PUTTING IT ALL TOGETHER

The sample experiment report that follows covers the ISMG criteria. Use this as a model for reference.

TABLE 3 Sample calculations—Data processing strategy involves the following calculations and the results of this processing are tabulated in Table 4

Calculation	Example using 48 g/100 ml KCl
Average $\frac{\text{(sum of all values)}}{\text{amount of values}}$	$= \frac{77.0 + 75.5 + 78.0 + 74.5 + 77.5}{5} = 76.5°C$
Uncertainty of the mean $\frac{\text{maximum trial} - \text{minimum trial}}{2}$	$= \frac{78.0 - 74.5}{2} = 1.75$
Percentage uncertainty of the mean (%) $\frac{\text{uncertainty}}{\text{average}} \times 100$	$= \frac{1.75}{76.5} \times 100 = 2.29\%$ (2dp)
Percentage error (%) $\frac{\text{experimental value} - \text{expected value}}{\text{expected value}}$	$= \left\lvert \frac{(76.5 - 67.5)}{67.5} \right\rvert \times 100 = 13.33\%$ (2dp)
Percentage measurement uncertainty (%) (Thermometer) (calculated using lowest average temperature, 76.5°C) $\frac{\pm 0.5°C}{\text{average}} \times 100$	$= \frac{\pm 0.5°C}{76.5} \times 100 = 0.7\%$ (1dp)

TABLE 4 Processed data

Concentration of KCL (g/100 ml)	Average temperature (±0.5°C) (1dp)	Theoretical temperature values for KCl (°C)	Uncertainty of the mean (2dp)	Percentage uncertainty of the mean (2dp)	Percentage error (2dp)	Percentage measurement uncertainty (1dp)
36	36.8	26	1.25	3.40%	41.54%	1.4%
40	49.9	40	2.00	4.00%	24.75%	1.0%
44	65.1	55	1.75	2.69%	18.36%	0.8%
48	76.5	67.5	1.75	2.29%	13.33%	0.7%

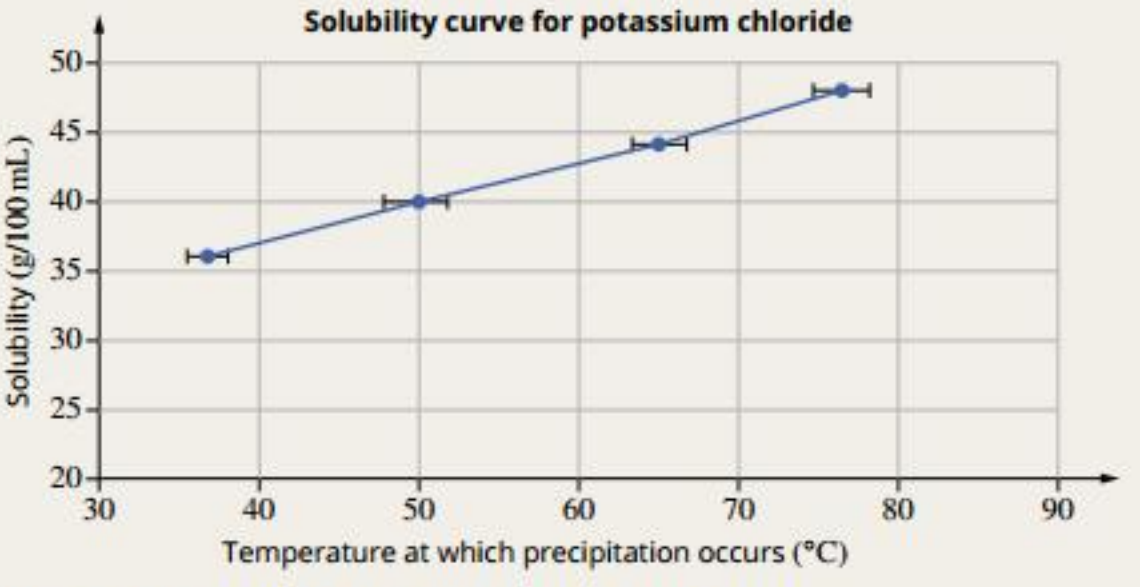


FIGURE 5 Solubility curve of KCl using the average values with error bars (± uncertainty).

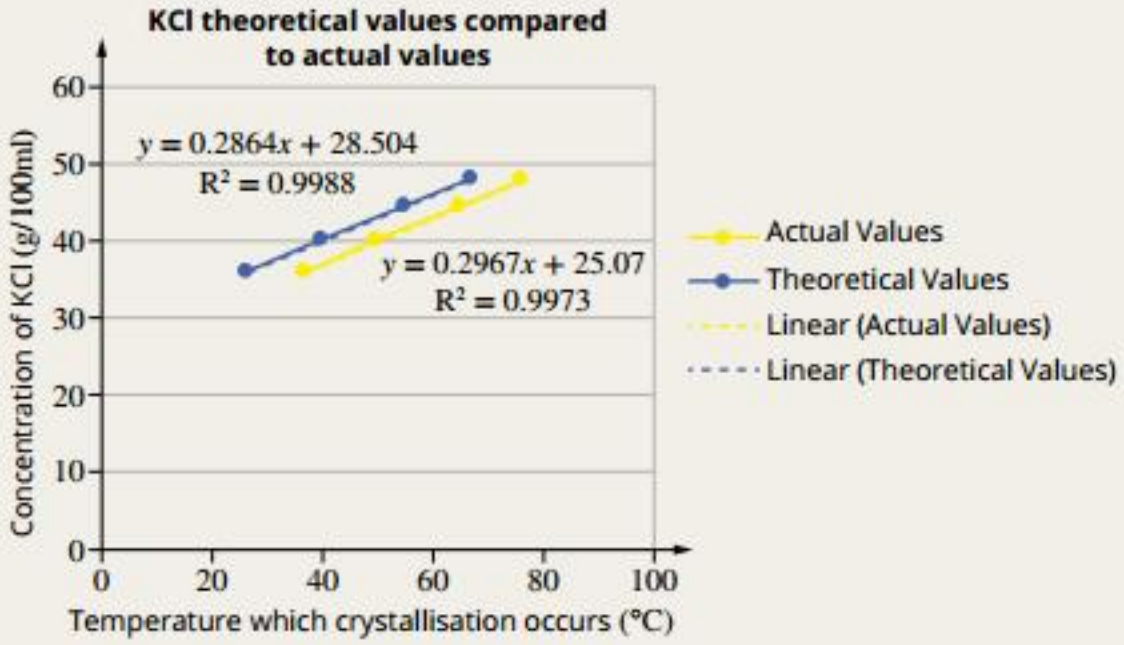


FIGURE 6 KCl theoretical values compared to derived data (Wikipedia, 2022).

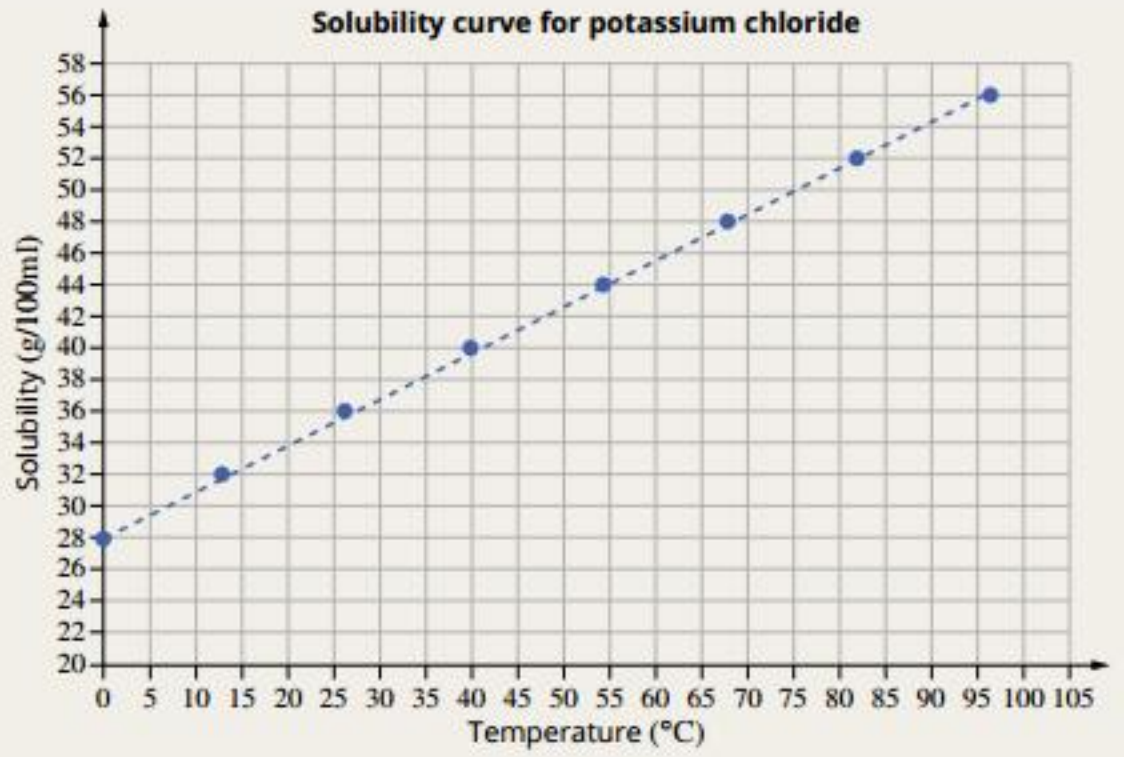


FIGURE 7 KCl theoretical values (Wikipedia, 2022).

Analysis

The solubility trend observed for KCl was that as concentration increased, so did the temperature of crystallisation. Figure 5 illustrates this pattern: precipitation occurred at 36.8°C for 36g/100mL and rose notably to 76.5°C for 48g/100mL. These findings are similar to theoretical values (Figures 6 and 7), although experimental temperatures were higher than theoretical values for each concentration used. This means that measured solubilities were lower than expected for all concentrations. The data displayed a strong linear trend with R^2 value exceeding 0.99.

Uncertainty of the mean was minimal, ranging from 2.29% to 4.00%, indicating low random error and precise experimental data as the values were all below 5%. This indicates reliable data. Non-overlapping error bars in Figure 5 suggest the averages are significantly different. Measurement uncertainty of the thermometer was also minimal, ranging from 0.65% to 1.36%.

However, data contains limitation(s) because accuracy was compromised by substantial discrepancies between theoretical and actual results, with percentage errors ranging from 13.34% to 41.54%. This hints at systematic errors in experimental design, potentially affecting data validity and limits its use in answering the research question. Additionally, the narrow concentration range tested (36g/100mL to 48g/100mL) could limit the generalisability of findings, a point to be explored further in the evaluation. There was only a 3.6% difference in the gradients of experimental vs theoretical datasets indicating the systematic error that was present changed little throughout the experiment.

1.12 Interpreting and evaluating

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- formulate a conclusion linked to the research question using interpretation of evidence
- justify your conclusion
- evaluate reliability and validity and justify your arguments with evidence
- suggest improvements and extensions

In order to be awarded a 5 for Interpreting and Evaluating you need to present a justified conclusion, justified discussion of the quality of the experimental process and suggest improvements and extensions derived on the analysis of the evidence.

JUSTIFIED CONCLUSION LINKED TO THE RESEARCH QUESTION

While you have already described the trend observed in the data (Analysis) it is important, in the conclusion, to extend this idea further to relate specifically to the research question. In an objective and clear manner, state the observed relationship between the dependent and independent variables using the terminology of the research question. Consider the following:

- was the research question supported?
- has the research question been fully answered? (If not, identify why not)

Table 1.12.1 shows examples of concluding statements.

TABLE 1.12.1 Strong and weak conclusions to a research question and hypothesis

	Strong conclusion	Weak conclusion
Research question: How does the temperature affect the pH of water?	Analysis of the results on the effect of an increase in temperature of water from 5°C to 40°C showed an inverse relationship in which the pH of water decreased from 7.4 to 6.7. These results support the current knowledge that an increase in water temperature results in a decrease in its pH.	The results show that temperature does affect the pH of water.
Hypothesis: An increase in the temperature of pond water will result in a decrease in the measured pH of the water sample.	An increase in temperature from 5°C to 40°C resulted in a decrease in the pH of the water from 7.4 to 6.8.	The pH of water decreased as temperature increased.

There are several ways to justify the conclusion including but not limited to:

1 describing the chemical concepts (scientific understanding and theory) that explains the observed relationship.

The key finding should be explained within the right context, meaning the related chemical ideas, concepts and theories. Does the data support the literature or contradict the literature? Within this context, explain the basis for the trend observed.

2 describing the evidence that led to the data trend.

State values that indicate the strength of the relationship between the experimental variables (data, observations or results) including information gained from the error bars on the graph and the R^2 value(s). Refer to your tables/graphs to cite evidence.

3 comparing your findings to secondary data you have found from journal articles or other reliable sources that are directly connected to the experiment.

Explain if the results support your observations. You should report that your results are consistent with the findings. Otherwise, it is essential that you reflect on the contrasting results and identify or suggest possible explanations why the results differ. This could be due to differences in the measurement technique or other factors such as the control or measured variables. It might also help you identify possible sources of error within your investigation.

In circumstances where a clear trend is not discernible, you can interpret what the results mean. Interpretations are made when limitations exist related to the methodology employed, the sample size, the instruments used, the variables controlled and the raw data measured. Interpretations are not meant to provide answers and comprehensive explanations, only a valid and reliable plausibility based on what was measured.

In the conclusion, it is appropriate to briefly describe evidence relating to the quality of experimentation and any key limitations. You have two aspects (already identified in Analysis), reliability and validity (as described by % uncertainty and % error, respectively). Describe which of these was high/low and what this indicates about reliability and validity. Resist the temptation to explain these further as this is more usefully done in the Evaluation.

The conclusion is sometimes positioned after the analysis and sometimes at the end of the report. Its placement in your report will need to make sense to you and maintain the flow of ideas:

- Option 1: planning → data collection and analysis → conclusion → evaluation
- Option 2: planning → data collection and analysis → evaluation → conclusion

JUSTIFIED DISCUSSION OF RELIABILITY AND VALIDITY

Your analysis and conclusion have identified the trend in the data but also identified two other key aspects of the data—reliability and validity. A statement of these has also been made in the conclusion. The verb in analysis is 'identify' but here (in Interpreting and Evaluating) the cognition is 'discuss'. This means that you must explain statements made in the analysis related to % uncertainty (reliability) and % error (validity). In your discussion, consider the following:

- are these low or high?
- what is the effect on the usefulness of the data to answer the research question?
- what could have caused excessive uncertainty and random error?
- what could have caused excessive systematic error?
- any factors that could affect validity, accuracy, precision and reliability of data.

As you consider this discussion, remember that your data processing has provided extensive evidence—not just the independent-dependent variable relationship but also measurement uncertainty, uncertainty of the mean and percentage error. Use these values to add depth to your discussion and use evidence rather than methodology to describe and discuss uncertainty and limitations in the investigation. For example, if you have calculated the percentage uncertainty associated with the measurement instrument (say, a measuring cylinder) to be 0.24% (see above), then suggesting that the lack of precision of this equipment is the cause of a percentage error of 40% is not reasonable.

A second example of the use of evidence relates to percentage error. If you have calculated the percentage error of the data to range between say 30% and 50% and also shown that the percentage error is decreasing during the experiment, your reasoning for the cause of this percentage error needs to relate to a factor which is less at the end of the experiment than at the beginning. An example of this is a Galvanic cell experiment where an electrode becomes slightly oxidised in the electrolyte solution during the experiment—the resistance of the circuit increases with oxidation. As a result, we expect the systematic error to increase during the experiment and so percentage error should increase not decrease. A proposed systematic or random error should be evident in the data for the syllabus descriptor 'justified discussion of validity' to be met.

As you discuss factors affecting the quality of the data, remember the definitions of random and systematic error and describe each factor in terms of one of these. Is the factor expected to always produce a change in the same direction (systematic error, low validity)? Or will the factor produce a more random effect where the value is sometimes higher and sometimes lower (random error, low reliability)? Look carefully at the evidence in your data for each of these. Refresh your understanding of random and systematic error using Figure 1.12.1.

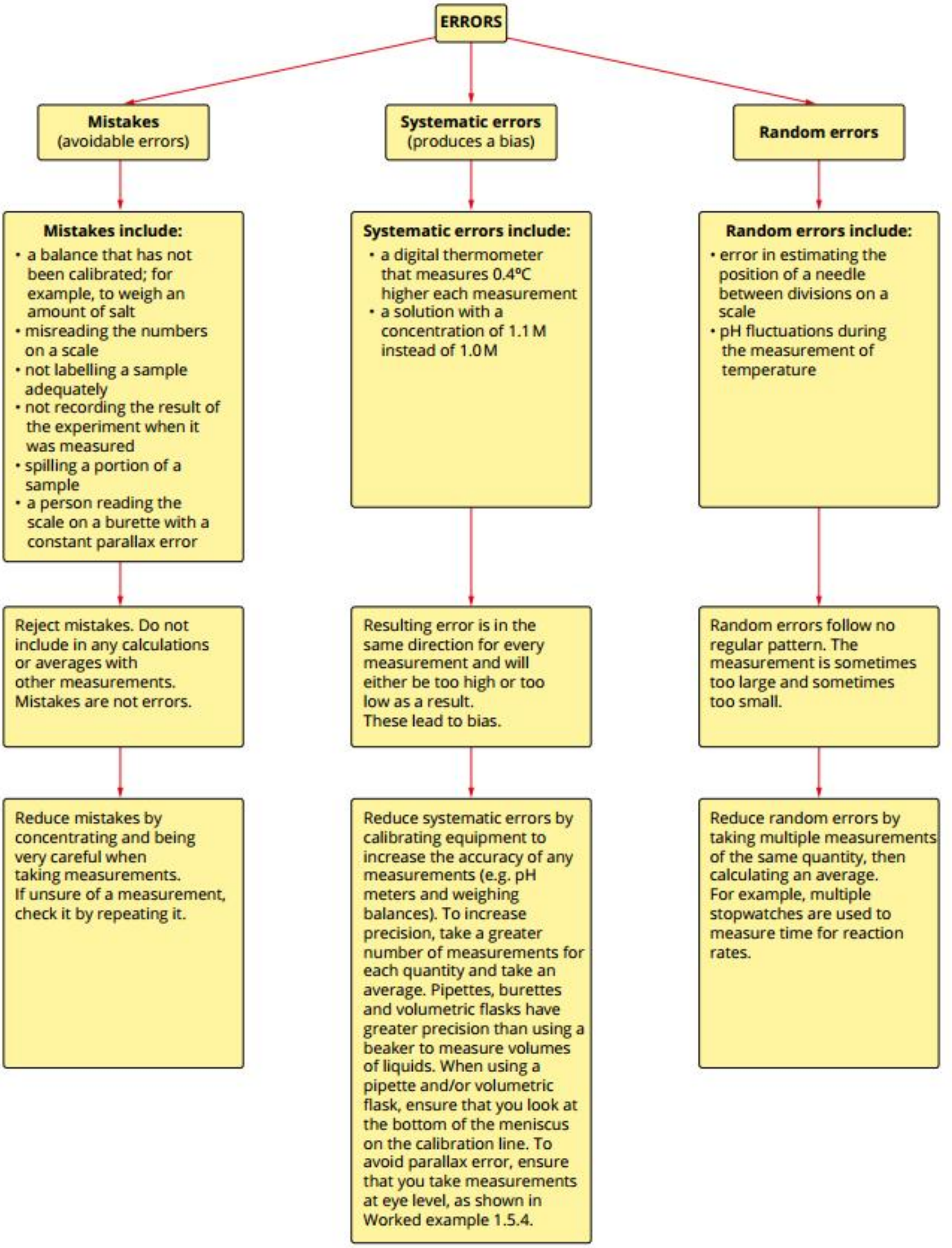

ERRORS
Mistakes
(avoidable errors)
Systematic errors
(produces a bias)
Random errors
Mistakes include:
• a balance that has not been calibrated; for example, to weigh an amount of salt
• misreading the numbers on a scale
• not labelling a sample adequately
• not recording the result of the experiment when it was measured
• spilling a portion of a sample
• a person reading the scale on a burette with a constant parallax error
Systematic errors include:
• a digital thermometer that measures 0.4°C higher each measurement
• a solution with a concentration of 1.1 M instead of 1.0 M
Random errors include:
• error in estimating the position of a needle between divisions on a scale
• pH fluctuations during the measurement of temperature
Reject mistakes. Do not include in any calculations or averages with other measurements. Mistakes are not errors.
Resulting error is in the same direction for every measurement and will either be too high or too low as a result.
These lead to bias.
Random errors follow no regular pattern. The measurement is sometimes too large and sometimes too small.
Reduce mistakes by concentrating and being very careful when taking measurements.
If unsure of a measurement, check it by repeating it.
Reduce systematic errors by calibrating equipment to increase the accuracy of any measurements (e.g. pH meters and weighing balances). To increase precision, take a greater number of measurements for each quantity and take an average. Pipettes, burettes and volumetric flasks have greater precision than using a beaker to measure volumes of liquids. When using a pipette and/or volumetric flask, ensure that you look at the bottom of the meniscus on the calibration line. To avoid parallax error, ensure that you take measurements at eye level, as shown in Worked example 1.5.4.
Reduce random errors by taking multiple measurements of the same quantity, then calculating an average.
For example, multiple stopwatches are used to measure time for reaction rates.

FIGURE 1.12.1 Types of errors that can be made in an experiment.

One form of systematic error is **bias** in sampling or measurements. Bias can result from poor definitions, incorrect assumptions, misunderstandings between group members and failure to use equipment correctly. Some biases cannot be eliminated but should at least be addressed in the discussion.

IMPROVEMENTS AND EXTENSIONS

Once any limitations or problems in the methodology have been identified, recommend improvements for how the investigation could be conducted if repeated. Some guiding questions are:

- has my research question been fully answered and what evidence is further required to answer it?
- what improvements can be made to aspects of the investigation identified as limitations?
- what changes to the materials or method would address the lack of reliability or validity of the data?

Questions to consider when suggesting extensions to this student experiment could include the following:

- do the findings lead to further questions?
- can the findings be extended to another situation?
- what extensions can be investigated for a related scientific idea?
- do the experimental findings have broader or further practical implications?

In the Modifications section, you provided a reason for each change that you made to the original experiment. In a similar way, provide a reason for each improvement and extension. In order to demonstrate that the extensions are logically derived from the analysis of the evidence, you need to provide a reason for each extension and how it relates to the evidence. Similarly, how the suggested improvements would have addressed or overcome the limitations that were identified earlier. Statements such as 'test more substances' or 'complete more trials' do not match a high-level response ('logically derived' ISMG descriptor) and will better match lower descriptors ('related' or 'ineffective').

The syllabus descriptor states 'logically derived' and so it is important to limit your suggestions for improvements and extensions to experimental issues that have already been identified (in analysis and evaluation). Conversely, if you have described a key limitation of the experiment related to high levels of random or systematic error, you should describe improvement(s) for this issue.

PUTTING IT ALL TOGETHER

The sample experiment report that follows covers the ISMG criteria. Use this as a model for reference.

Conclusion

It was found that increasing concentrations of KCl (36 g/100 ml, 40 g/100 ml, 44 g/100 ml and 48 g/100 ml) correspondingly raised the temperature at which crystallisation took place (see Figure 5). For instance, precipitation occurred at 36.8°C with a KCl concentration of 36 g/100 ml, and at 76.5°C with 48 g/100 ml. This trend is due to increased thermal energy at higher temperatures which increases particle movement, which in turn increases collisions between particles of solute and solvent and weakens existing bonds between particles. Specifically, water molecules, due to their polarity, attract ions from KCl, causing its cations and anions to separate at higher temperatures. Upon cooling, the reduced kinetic energy prompts crystallisation of the solute as ions have less movement and greater ability to reform ionic bonds between K^+ and Cl^- (lattice reforms).

The experiment exhibited high reliability (2.29%–4.00% uncertainty, low random error) but low validity (13.33%–41.54% error, high systematic error). Thus, addressing limitations (mostly systematic error) is crucial for accurately answering the research question.

Evaluation

The method employed in this experiment demonstrated reliability, evidenced by consistently low percentage uncertainty and measurement uncertainty (Table 4). This indicates minimal random error and suggests

reproducibility of results by other researchers. To further reduce uncertainty, expanding the range of samples could help refine data and identify outliers.

However, the method's validity is compromised by significant percentage errors ranging from 13.33% to 41.54%, particularly notable at 36 g/100 ml of KCl (41.54%). All temperatures recorded were higher than expected—this means that KCl in the current experiment showed solubilities lower than expected. As the gradients of the trend lines were similar, there is evidence of systematic error(s). This could possibly be due to challenges in determining complete dissolution in the water bath—if the solution still contained undissolved crystals at the start of the experiment, crystallisation could be accelerated. Also, it was difficult to see the small crystals as they were appearing because the test tube had water on the outside. However, this difficulty is unlikely to have caused the systematic error of a too-high temperature because the difficulty in seeing the crystals would likely cause a too-low temperature reading due to a delayed reaction time in recognizing crystallisation. Other inconsistencies could have resulted from varying times the tubes were in the water bath and so varied evaporation levels among test tubes. This might influence concentration and subsequent precipitation temperatures unpredictably.

Improvements and extensions

To improve this experiment, a dark paper background could be used during dissolving and also during crystal detection to make sure the solute is first fully dissolved and secondly detected at the correct time. Additionally, to avoid excess evaporation while in the water bath, immersion times for test tubes should be standardised and a loose stopper used, thereby improving methodological reliability and data accuracy.

Furthermore, the limited range of concentrations (four tested concentrations) limits the full identification of the trend. Increasing the number of concentrations would provide a more comprehensive dataset, enabling more confident trend analysis and better comparison with theoretical values.

A suitable extension to this investigation would be to investigate the solubility of a potassium compound with an even larger anion (e.g. $MnO4^-$). Comparing the current data to the original experiment shows that decreasing the size of the anion (NO_3^- to Cl^-) decreases the solubility. This trend could be due to steric hindrance within the lattice—the lattice is stronger when the anion and cation are about the same size (Holmes et al. 2019). KCl is shown to have a lower solubility than KNO_3—using this trend we would expect $KMnO_4$ to have a higher solubility than both KCl and KNO_3. On the other hand, determining the solubility curve for lead nitrate or sodium nitrate could further explore the effect on solubility of changing the cation (not anion) in an ionic compound.

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PART C RESEARCH INVESTIGATION (IA3)

The research investigation assessment requires students to investigate a claim, provided by their teacher, by drawing on secondary evidence from scientific texts. Students will draw on research to analyse, interpret and evaluate the evidence to reach a justifiable conclusion about the research question. The task requires students to locate and use information beyond the scope of their knowledge and data they have been given.

QCAA Syllabus states that students must work individually to develop and investigate their own research question.

The research investigation constitutes 20% of the total subject score and may be presented in:

- written form of up to 2000 words, or
- multimodal form using at least two modes delivered simultaneously and up to 11 minutes.

INSTRUMENT-SPECIFIC MARKING GUIDE

As with the Student experiment, responses are assessed against an instrument-specific marking guide (ISMG). In developing the research report, it is important to keep in mind the assessment objectives, particularly the characteristics that are described in the performance level descriptors.

The ISMG has four criteria: Forming and finding, Analysing, Interpreting and Evaluating.

Each criterion has performance levels, against which the qualities of the response are assessed.

A performance level is comprised of a performance level descriptor and mark (or range of marks).

The performance level descriptor describes the characteristics that are demonstrated by a response of that quality.

In this part, each stage of the development of the research investigation will be discussed and aligned with the relevant ISMG criteria, and elaborations for the highest performances.

The research question should specifically address one of the concepts associated with the claim. Commence by identifying a claim and developing your own research question based on that claim. Since this assessment relies heavily on access to research, students need to be able to easily find sources relevant to the research question. Throughout the process, be mindful that scientific language and representations are used (Refer to Module 1.8).

1.13 Forming and finding

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand and select a claim
- classify elements of the claim
- unpack the elements to identify variables, terms and concepts related to the claim
- plan research and locate sources relevant to the claim
- distinguish between primary and secondary sources
- locate a range of primary and secondary sources
- use a scientific journal to record the information in the sources
- refine the concepts to develop an investigable research question
- understand the criteria against which the research investigation will be assessed.

The ISMG for the Forming and finding criterion, shown in Table 1.13.1 below, is assessed in relation to the development of the research question from the claim and the communication of the findings of the investigation through a scientific report.

TABLE 1.13.1 The performance characteristics associated with the highest performance level of the Forming and finding criterion

Criteria	Assessment objectives	Performance Characteristics	Marks
Forming and finding	1. Describe ideas and findings about the properties and structure of organic materials or chemical synthesis and design. 2. Apply understanding of the properties and structure of organic materials or chemical synthesis and design to develop research questions. 6. Investigate phenomena associated with the properties and structure of organic materials or chemical synthesis and design through research.	• a considered rationale identifying clear development of the research question from the claim • a specific and relevant research question • selection of sufficient and relevant sources • appropriate use of genre conventions • acknowledgment of sources of information through appropriate use of referencing conventions	5

There are three aspects to the Finding and forming criterion.

To achieve the highest mark (5) in the Forming and finding criterion, you need to create a research question clearly linked to the Unit 4 subject matter that identifies measurable independent and dependent variables, as well as a control variable-specific research question. Then you need to construct a rationale that clearly outlines how the research question is developed from the original claim. A research rationale outlines the reason to conduct research on your chosen claim i.e. it is the justification for the investigation. This is achieved by conducting a thorough literature review to understand what is already known in the chosen topic and to identify the concepts from Unit 4 that are related to the topic. Students who explain concepts outside the syllabus in their Rationale struggle to stay within the word limit.

Finally, the structure and style of the report, quality of sources and use of referencing are assessed.

UNDERSTANDING THE NATURE OF A CLAIM

A claim is an assertion made without any accompanying evidence to support it. The claim can be a sentence, statement within a sentence, title of an article, quote or anything published in any form. The claim should be in isolation from any justification using data, research, evidence or reasoning from known information to support it. The claim is a broad statement that can encompasses a range of related topics and relationships.

SELECTING A CLAIM

If you are provided with a choice of claims, you should ask yourself the following questions about the claims.

Which claims:

- interest me or are most relevant to me?
- are easy to break down and link to the subject matter in the unit?
- are broad enough to allow me to undertake a unique investigation?

The answers to these questions will help you decide on the most appropriate claim for you.

To develop the research question from a claim, students must analyse, understand and identify one or more of the following:

- known scientific concepts
- variables
- measurable terms
- ideas related to concepts
- a term that is stated to influence another.

Record the information you collect, your thoughts and your analysis in a hard copy or electronic scientific journal. When you write the report, this information will be useful in writing the rationale that documents how the research question was developed from the claim. Write down all the elements found in the claim and try to categorise them using the list above. Each element within the claim may suit more than one category. Table 1.13.2 outlines an example of analysing and categorising elements of a claim.

TABLE 1.13.2 Three examples of analysing and classifying elements of a claim

Example Claim 1: Plastics are bad for the environment		
Elements	**Classifying elements of the claim**	**Unpacking the elements**
• Plastics are made from crude oil.	• a term that is stated to influence another	• hydrocarbons
	• a term that is stated to influence another	• polymers
	• ideas that relate to concepts	• non-renewable resource
	• measurable terms • variables	• manufacture requires lots of resources/energy
• Plastics are disposed of and not recycled.	• known scientific concepts	• all plastics can be recycled but not all are waste
• Plastics release toxic chemicals.	• ideas that relate to concepts	• breakdown in environment
	• known scientific concepts	• chemicals released from combustion additives
• Plastics are not biodegradable.	• measurable terms	• polymers are inert
	• ideas related to concepts	• not easily broken down in nature by air, water, sunlight

Example Claim 2: Natural shampoos are better than commercial shampoos		
Elements	**Classifying elements of the claim**	**Unpacking the elements**
• Define the term 'better'.	• measurable terms • variables	• more environmentally friendly
	• ideas related to concepts • variables	• better cleaning efficiency
• Natural shampoos do not contain harmful chemicals.	• a term that is stated to influence another	• synthetic chemicals are toxic
• Natural shampoos clean as effectively as commercial shampoos.	• known scientific concepts	• how surfactants work
	• measurable terms • known scientific concepts	• cleaning effectiveness is measurable and related to surface tension, wetting time, solid content, foaming ability

Example Claim 3: Green chemistry is clean chemistry.		
Elements	**Classifying elements of the claim**	**Unpacking the elements**
• Green chemistry	• a term that is stated to influence another	• green solvents
	• ideas related to concepts	• preventing pollution
	• ideas related to concepts	• renewable energy
	• a term that is stated to influence another • measurable terms • variables	• atom economy—more effective synthetic reaction
	• a term that is stated to influence another.	• renewable materials
• Environment	• measurable terms • variables	• fewer pollutants released
	• measurable terms • variables	• fewer resources required
• Clean chemistry	• ideas related to concepts	• non-toxic
	• measurable terms • variable	• less energy required
	• measurable terms	• reduced reagents

LOCATING SOURCES

It is important to recognise that this is not a university quality report as students do not have the time, access or understanding to analyse the information provided in the scientific research journals. In addition, the research investigation is limited to 2000 words, so does not allow for the depth of investigation in a research journal.

When gathering scientific evidence for the research investigation, source it from reputable publications including:

- scientific journals: research papers and scientific reviews
- scientific articles written by organisations who apply scientific research to their industry
- commercial articles such as science magazines, newspapers and also websites.

The research investigation must include a reference list of sufficient and relevant sources. *Sufficient* is defined as 'enough or adequate for the purpose', and *relevant* as 'bearing upon or connected with the matter in hand; to the purpose; applicable and pertinent; having a direct bearing on'. Figure 1.13.1 points out the features of sources deemed *sufficient* and *relevant*.

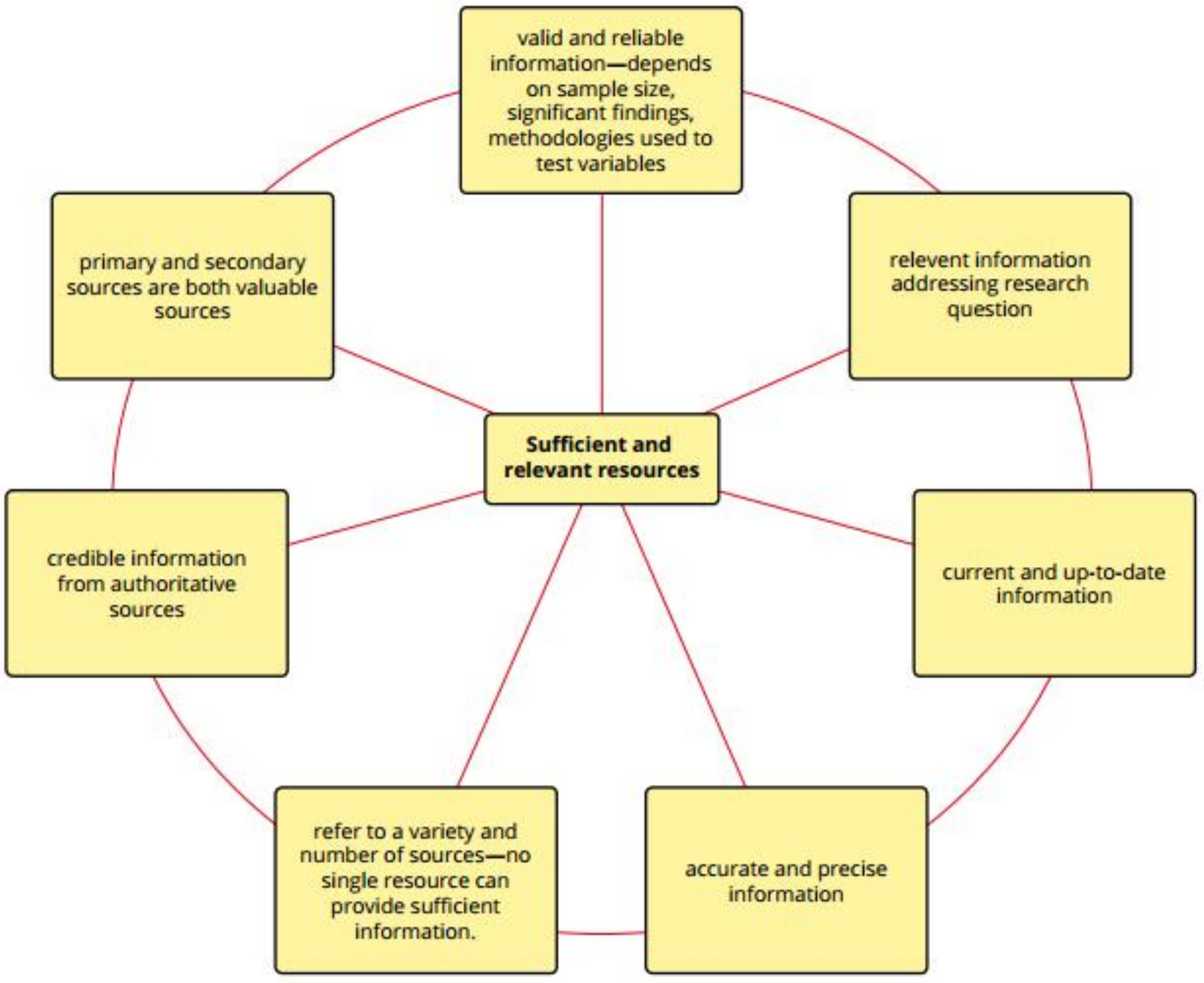
valid and reliable information—depends on sample size, significant findings, methodologies used to test variables
primary and secondary sources are both valuable sources
relevent information addressing research question
Sufficient and relevant resources
credible information from authoritative sources
current and up-to-date information
refer to a variety and number of sources—no single resource can provide sufficient information.
accurate and precise information

FIGURE 1.13.1 Features of sources suitable for the research investigation.

A good place to start research is to look for interesting sites and textbooks to identify relevant keywords and concepts rather than immediately searching for complex research articles. This could include videos, general scientific articles and even Wikipedia to gain a general understanding of the topic.

Access available open-access sources, some of which can be identified using Google Scholar, educational, government or industry websites, with suffixes including .edu, .gov or .org

Where necessary, you can often freely access scientific journals through academic networks, such as ResearchGate and Academic.edu. If the article has not already been published, you can request a copy of the article from the author or ask them a question.

When accessing the sources, start with the title, which should include some of the keywords related to the concept. As you refine the focus of your investigation, use the evidence to refine the claim and develop the rationale. Your search will narrow and lead to data tables, graphs, images and abstracts. If the abstract is useful, download the article or request a copy of it. Look at the images and conclusion. These may be more useful than the text of the article.

Remember to document the sources and summarise the information contained in your journal to facilitate the writing of the report and generate a reference list.

A useful way to collate the evidence is in a table with headings such as:

- Article overview, which summarises the article
- Evidence, which outlines the methodology, trends/patterns/relationships and limitations
- Conclusions, which summarises the evidence
- Relationship to research question, which includes your thoughts and highlights the parts of the research question that this evidence addresses
- Limitations, which identifies aspects of the research question that are not addressed or cannot be answered due to the methodology

Consider whether the information you use is from a primary or secondary source.

Primary and secondary sources

Table 1.13.3 summarises the characteristics of primary and secondary sources. Sometimes the same information may be contained within a primary and a secondary source, depending on when and by whom it was written. For example, a scientist's journal article on a clinical trial of treatments for teenage obesity is a **primary source**, while a general magazine article about teenage obesity, written by a journalist and referring to the scientific study, is a **secondary source**.

TABLE 1.13.3 Summary of primary and secondary sources

	Primary sources	Secondary sources
characteristics	• first-hand records of events, experiences, experimental data • written at the time the event happened • original documents	• interpretations of primary sources • written by people who did not see or experience the event • use information from original documents but rework it
examples	• results of experiments • scientific journal/magazine articles • reports of scientific discoveries • photographs, specimens, maps and artefacts • interviews with experts • websites (if they meet the criteria above)	• textbooks • biographies • newspaper articles • magazine articles • radio and television documentaries • websites that interpret the scientific work of others • podcasts

A primary source is written by the observer/witness of an event or the scientist who conducted the research. The information has only been processed by the original observer; therefore, it is the least biased of all available sources of information. However, even primary sources may be biased, as the observer or researcher had to make choices related to the observation, control of variables, use of instruments and choices for processing data.

Secondary sources of information are not eyewitness accounts but interpretations of events by other people. As second-hand information, accuracy and reliability may be reduced, and events may be interpreted through the writer's perception and bias. You should aim to use a wide range of data sources when using secondary data, to cross-check for accuracy, reliability and validity of information.

When searching for information and evidence, follow these guidelines.

1 Determine if it is a primary or secondary resource.
2 Confirm that it is valid.
   a Check that it contains information that is specifically related to the claim.
   b Check that the evidence and information are pertinent to the variables in the research question.
3 Assess its reliability.
   a Is it current/recent information?
   b Is it up-to-date in its understanding of relationships?
   c Is the evidence equivalent to other sources?
   d Check credibility—consider who the author is, their qualifications and expertise.
   e Evaluate the methodology, including what variables were controlled or measured.

Articles in scientific journals

Peer-reviewed scientific journals are excellent sources of information. Journals are a collection of scientific reports written by scientists who conducted research. The reports and articles found in scientific journals are published primary sources, meaning they are the results of the experiments (Figure 1.13.2).

Polymer Chemistry

PAPER

Cite this: Polym. Chem., 2024, 15, 2070

Solvent effects on surface-grafted and solution-born poly[N-(2-hydroxypropyl)methacrylamide] during surface-initiated RAFT polymerization †

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rsc.li/polymers

The difference in the molar mass between surface-grafted and solution-born polymers grown during surface-initiated (SI) polymerization has caused controversy for years. To understand it, we study the solvent effects on the polymer formed on the surface and in the solution by investigating their macromolecular parameters. We utilized reversible addition fragmentation chain-transfer (RAFT) polymerization to grow surface-grafted and solution-born poly[N-(2-hydroxypropyl)methacrylamide] (p(HPMA)) under different solvent conditions. Changing the solvent proticity and/or polarity in fluences the solution propagation rate, leading to mass transfer limitations and a concomitant discrepancy in the molar masses of the polymer formed in solution and grafted from the surface. Moreover, the solvent effects were found to directly determine the grafting density of surface-grafted p(HPMA). These results highlight how decisive the solvent effects on the SI-RAFT polymerization of HPMA are and that they may be key to regulate the physical and macromolecular parameters of the obtained surface-grafted p(HPMA) brushes.

Introduction

Poly[N-(2-hydroxypropyl)methacrylamide] (p(HPMA)) represents the state of the art of biocompatible, non-toxic, and non-immunogenic polymers and has found extensive use in drug delivery.[1–4] Its polymer brush coatings on surfaces inhibit non-specific protein binding (fouling) in various biomedical applications.[5–8] P(HPMA) brushes showed outstanding hemocompatibility and prevented surface thrombogenicity under dynamic flow conditions.[6,9] In our previous study,[10] we reported that the antifouling performance of the p(HPMA) brushes increased with increasing grafting density of the polymer chains. Importantly, we showed how the selection of the grafting method directly affects the grafting density of the p(HPMA) coatings on the surface and that denser polymer brushes can be achieved by the grafting-from (GF) approach. Methods employed for GF typically rely on controlled radical polymerizations (CRP),[11,12] such as nitroxide-mediated polymerization,[13–15] atom-transfer radical polymerization (ATRP)[16–21] and reversible addition fragmentation chain-transfer (RAFT) polymerization.[22–28] In particular, surface-initiated (SI) RAFT polymerization is gaining increased attention due to its advantageous features, such as excellent monomer compatibility and lack of metal catalysts toxic to cells, which is beneficial for biomaterial applications.[29–31]

Besides the grafting density of the polymer brush, the molar mass of the polymer chains on the surface is also an important physical parameter influencing the coating's antifouling ability[32] but it is challenging to measure it directly.[33–35] The difficulty in accessing the molar mass distribution of surface-grafted polymer generated during SI polymerizations comes from the fact that its mass is extremely low, making analysis by typical methods such as size-exclusion chromatography (SEC) problematic. While some authors have assumed that the molar mass of the surface-grafted polymer is comparable with that of the polymer grown concomitantly in solution during the SI-polymerization,[36] experimental studies have demonstrated that the polymer molar mass on the surface and the solution-born polymers may be similar or differ greatly, depending on polymerization conditions.[37–39] Genzer's and Spencer's groups attributed this discrepancy to a phenomenon they termed "crowding" during SI-ATRP polymerization at high grafting density and/or with a high propagation rate.[40,41] Crowding limits mass transfer at the surface, slowing down

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† Electronic supplementary information (ESI) available. See DOI: https://doi.org/10.1039/d4py00177j

FIGURE 1.13.2 An extract of an article in a scientific journal of a research report written by scientists. It is strictly structured with a pertinent title, names of authors, an abstract, the report which uses the convention of: introduction, method, results, analysis, conclusion and ends with a reference list.

Access to scientific journals can be difficult as many journals require you to purchase a subscription or membership, though some are free. Figure 1.13.3 provides ideas for accessing scientific journals.

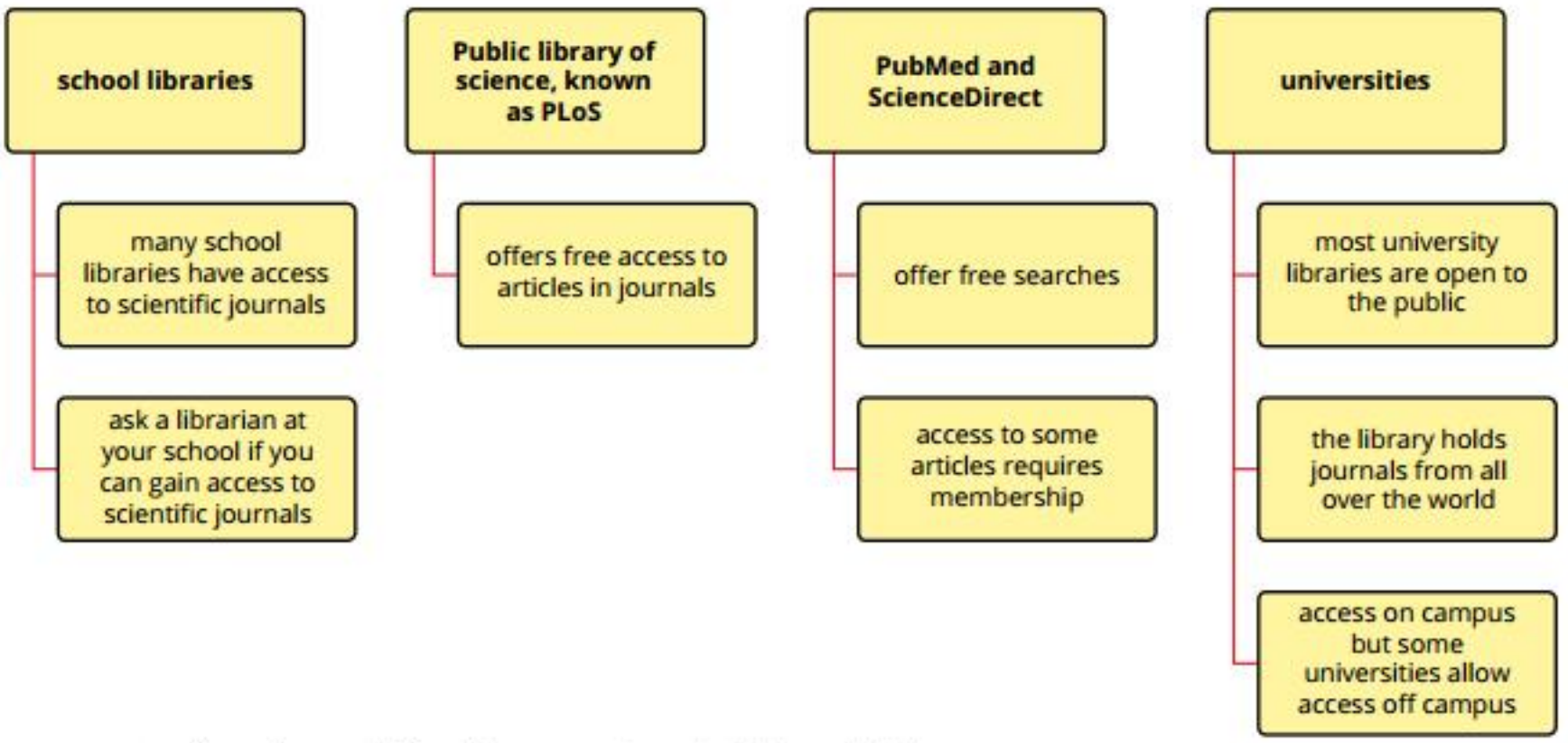

school libraries
many school libraries have access to scientific journals
ask a librarian at your school if you can gain access to scientific journals
Public library of science, known as PLoS
offers free access to articles in journals
PubMed and ScienceDirect
offer free searches
access to some articles requires membership
universities
most university libraries are open to the public
the library holds journals from all over the world
access on campus but some universities allow access off campus

FIGURE 1.13.3 Suggestions and information on accessing scientific journal articles.

Scientific articles are excellent sources of information but also have their drawbacks as sources for the research investigation. Table 1.13.4 outlines some advantages and disadvantages of sourcing and using articles in scientific journals for the research investigation.

TABLE 1.13.4 Advantages and disadvantages of scientific articles

Advantages	Disadvantages
• written by experts • authoritative information (peer-reviewed) • most current information • logical, organised layout • content is relevant to the topic • contains an abstract that summarises all information in the article (if you don't find the information in the abstract, the article is not relevant) • primary source • provides introductory comments that review the literature of the field and position of the research focus of the article in it.	• information is complex and challenging to understand • complex language and advanced processing and analysis of data • requires a high level of scientific literacy, language and numeracy to understand • may be time consuming to read and analyse • well-established concepts do not have recent published articles • may be difficult to locate

FIGURE 1.13.4 A science magazine you might find in your school library.

Books and physical publications

Secondary sources such as good science magazines and books are valuable sources of secondary information.

The first source you should use is your textbook. The language and concepts are presented specifically for high school students. In addition, the textbook addresses the syllabus objectives. Non-fiction books and magazines will probably be commonly used resources for the research investigation. Common commercial science magazines you might find in your school library include *The Helix*, *Cosmos*, *Scientific American* and *New Scientist* (Figure 1.13.4). Table 1.13.5 outlines some advantages and disadvantages of non-fiction books as sources for your research.

TABLE 1.13.5 Advantages and disadvantages of book resources

Advantages	Disadvantages
• may be written by experts • potentially authoritative information • logical, organised layout • content is relevant to the topic • contain table of contents and index to help find relevant information • easily located in libraries • written in language that is understandable	• may not have been published recently • usable by only one person at a time • may have more bias than primary sources

Searching online

Online sources include online scientific organisations such as CSIRO, NCBI, AIMS, Bioscience (Oxford Academic) and other university publications and press. Many government and privately funded science organisations publish material, along with not-for-profit scientific organisations. Websites may direct you to magazines and scientific journals (such as those described above), the news, podcasts, blogs and videos (institutional, company and personal).

Information located on the internet requires very careful scrutiny. The openness and ease of publishing on the internet means information may not be valid and reliable. Use the earlier guidelines to help you evaluate sources. Table 1.13.6 outlines advantages and disadvantages of locating and using information online.

When searching for relevant information, you need appropriate search terms to enter into a search engine. These tips can help your search.

- Break your search statement into concepts and key words.
- Find synonyms, other related terms and concepts that apply to the topic.
- Create concepts of 1–3 words to enter into the search engine.
- Try different combinations of terms.
- Do not settle for the first sites on the list or your first attempt—look beyond the first page of results.
- Look through the results for sites from science organisations and research institutions (e.g. CSIRO, WEHI, NIH; .gov, .org), universities (.edu) and science journals and magazines.

TABLE 1.13.6 Advantages and disadvantages of internet resources

Advantages	Disadvantages
• quick and easy to access • allows access to hard-to-find information • access to the whole world; millions of websites • information is potentially more up to-date • may be interactive and use animations to enhance understanding	• may not be reliable, valid or credible • can easily side track with non-relevant information • a lot of 'junk' sites and potentially more biased material • need to discern search engine results to find most useful sites • cannot always tell how up-to-date information is • can be hard to tell who has responsibility for authorship • information may not be well ordered

Overview of resources

Your textbook should be your first source of reliable information. Other information should be consistent with this. Articles published in journals and magazines often present findings of new research, which may or may not be confirmed later, so be careful not to treat such sources of information as established fact. Scientific journals are **peer-reviewed** (critically reviewed by other specialist scientists), which gives them more credibility than other sources.

However, it is important that the sources utilised in the investigations are credible and easily accessible.

FORMING A QUESTION

The claim is used to develop the research question investigated in the assessment. The variables inferred from the claim may not be measurable or directly observable, and therefore they may not be scientific.

To help to develop the research question, break the claim into possible scientific elements, each of which could be used to form a question (Table 1.13.7 on page e106). Separating the claim into elements, such as related terms and concepts, enables you to formulate variables, measurable items and questions. Thus, you can identify scientific elements of the claim that are contained in the syllabus.

Based on these elements, formulate a number of questions related to the claim and record all of them in the journal. The research question must specify a dependent variable and enable a response that will evaluate the validity or the reliability of the claim. You will need to understand the dependent and independent variables and the relationship between the variables. The research question must identify the dependent variable and may also specify the independent variable.

Some guidelines to help form a research question include:

- identifying a dependent variable that can be linked to the claim or rephrasing the claim into something measurable
- developing an element of the claim into the independent variable or identifying it in the stimulus material
- phrasing a question to ask if the independent variable will influence, cause or correlate with the dependent variable
- writing a few different questions.

Usually, the questions improve as you write more, which allows the formulation of a more developed research question. At this stage, these questions can still be quite broad but they will need to be refined; the focus of the research question needs to be very narrow so that the research report can be completed within the assessment conditions.

The process to developing a research question is often cyclical (Figure 1.13.5).

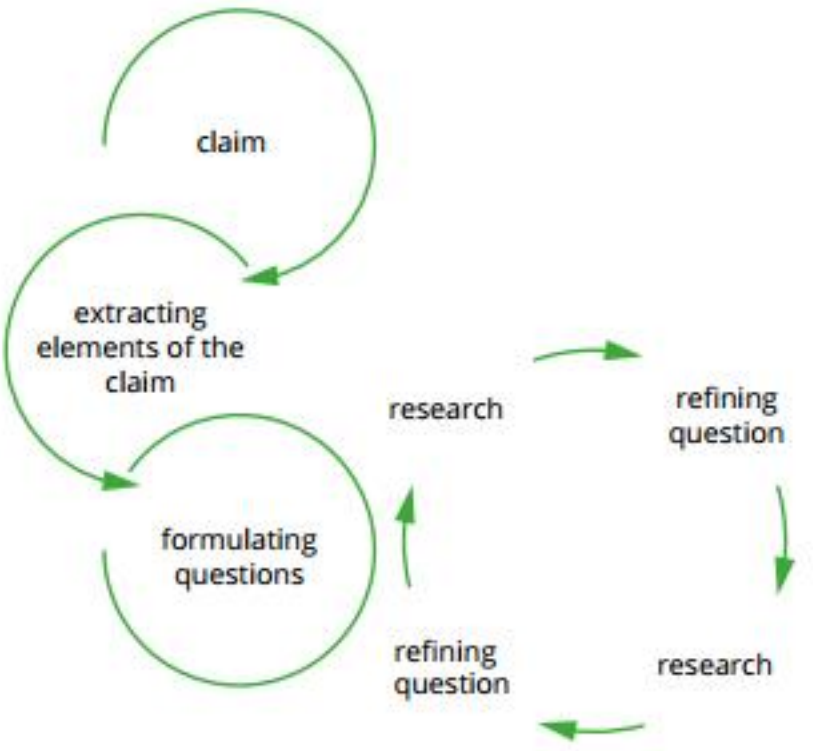


FIGURE 1.13.5 A chart of a common process for developing a research question. This cycle can be repeated as many times as necessary until a scientist is satisfied with the investigation question.

Read through Table 1.13.7 to see examples of questions formed from the elements of the claims that are refined.

TABLE 1.13.7 Three examples of questions formulated from a claim

Example Claim 1: Plastics are bad for the environment.		
Elements	**Elaboration of the claim**	**Formulated questions**
Plastics are made from crude oil.	About 4% of the world's crude oil is used to make plastic.	Can the efficiency of the distillation process be increased?
	Hydrocarbons are collected by distillation.	
	Non-renewable nature of the resource.	Can reactants in the plastics process be made from something other than crude oil?

Example Claim 2: Natural shampoos are better than commercial shampoos.		
Elements	**Elaboration of the claim**	**Formulated questions**
Natural shampoos clean as effectively as commercial shampoos.	Shampoo effectiveness can be evaluated by comparing the surfactant properties of the shampoos.	Does a greater reduction in the surface tension mean that the shampoo is more effective?
	Surfactants have a non-polar aliphatic chain and polar head.	Do natural shampoos work in the same way as synthetic shampoos?
	Properties: • surface tension • wetting ability • solid content • detergency • foaming ability	

Example Claim 3: Green chemistry is clean chemistry.		
Elements	**Elaboration of the claim**	**Formulated questions**
Green chemistry	Atom economy	Can the chemical yield of a reaction be increased?
		Does a higher atom economy mean a greener product?
		Is it possible to make the same product in different ways?

REFINING THE RESEARCH QUESTION

One of the questions in your journal will become your research question. As you conduct research into the independent and dependent variables, new information will refine the question so it is more specific.

Since the Forming and finding criterion assesses the development of the research question from the claim, it is important to record your development of conceptual understanding and the knowledge you gain about the relationships between variables.

Table 1.13.8 compares a formulated question with a developed research question. Always get the teacher to assess your research question.

TABLE 1.13.8 Development of the original questions formulated into research questions

Example Claim 1: Plastics are bad for the environment.		
Formulated question	**Refined research question**	**Variables**
Can the efficiency of the distillation process be increased?	If the number of stages within the fractional distillation tower is increased to collect fractions with a smaller temperature range, could polymers be made more environmentally friendly?	*Dependent:* Carbon footprint of the resulting polymers *Independent:* Number of stages in the distillation tower **OR** fraction size
Can reactants in the plastic process be made from something other than crude oil?	Can the monomers that are used to generate the plastics used in polyurethanes be generated from a renewable resource?	*Dependent:* Number of monomers *Independent:* Renewable resource

Example Claim 2: Natural shampoos are better than commercial shampoos		
Formulated question	**Refined research question**	**Variables**
Does a greater reduction in the surface tension mean that the shampoo is more effective?	Are natural shampoos better cleaners than synthetic shampoos based on the surface tension, wetting ability, solid content, detergency and foaming ability?	*Dependent:* Cleaning efficiency *Independent:* Shampoo type (natural/synthetic)
Do natural shampoos work in the same way as synthetic shampoos?	Do the chemicals in natural shampoos create micelles that have a non-polar aliphatic chain with a polar head that increase the solubility of the oily substances in water?	*Dependent:* Solubility of [choose a substance] *Independent:* Shampoo type (natural/synthetic)

Example Claim 3: Green chemistry is clean chemistry		
Formulated question	**Refined research question**	**Variables**
Can the chemical yield of a reaction be increased?	Would increasing the temperature in the Haber process to shift the equilibrium towards the products increase the overall greenness of the ammonia production process?	*Dependent:* Greenness of the Haber process *Independent:* Temperature
Does a higher atom economy mean a greener product?	Can improving the chemical yield of the synthetic reactions through higher atom economy create a greener manufacturing process?	*Dependent:* 'Greener' manufacturing process **OR** Chemical yield *Independent:* Atom economy
Is it possible to make the same product in different ways?	Can the polymers be made from non-petroleum sources to reduce the greenhouse gas emissions associated with petroleum production?	*Dependent:* 'The greenhouse gas emissions associated with plastic production *Independent:* Whether the polymers are made from non-petroleum sources

Your research investigation report requires a considered rationale for the research question, displaying its clear development from the claim. Outline this step-by-step development, justifying the steps using scientific concepts, knowledge and understanding.

Therefore, a research question must explicitly identify the dependent and independent variables. The research question must be connected to the considered rationale and the topic of study.

PUTTING IT ALL TOGETHER

The structure of the research report is not mandated by the assessment specifications but needs to be presented using appropriate report conventions, such as appropriate headings and language, and sources of information need to be acknowledged using referencing conventions.

Possible report structures include headings such as Claim, Rationale, Research question, Introduction or Background, Analysis and interpretation, Conclusion and Evaluation, or organised under the headings of the instrument-specific marking guide (ISMG) criteria as stated in the QCAA syllabus; Forming and finding, Analysing, Interpreting and Evaluating. However, you may elect to organise your report in a different but logical order.

As stated at the beginning of this module, the characteristics of the highest performance level indicate appropriate use of genre conventions and acknowledgment of sources of information through appropriate use of referencing conventions. Therefore, the report needs to follow the advice and directions presented in Module 1.8 from Part A.

The sample research investigation report that follows covers the ISMG criteria and may be used as a reference tool. Use this as a model for reference.

Forming and Finding

Claim

Biofuels are more efficient and have less environmental impact than fossil fuels.

Rationale

Climate change represents a considerable challenge of our era. Projections indicate that by 2100 the Earth's average temperature could increase by between 1.5 and 4°C (IPCC, 2014). This is consistent with other atmospheric circulation models and is primarily due to the rise in CO_2, a known greenhouse gas, from fossil fuel combustion (Figure 1, NASA, 2024) (United Nations, n.d). The combustion of fossil fuels makes up 90% of all CO_2 emissions. Biofuels, produced from plants, also produce carbon dioxide but as they are derived from photosynthesis, they are more carbon neutral.

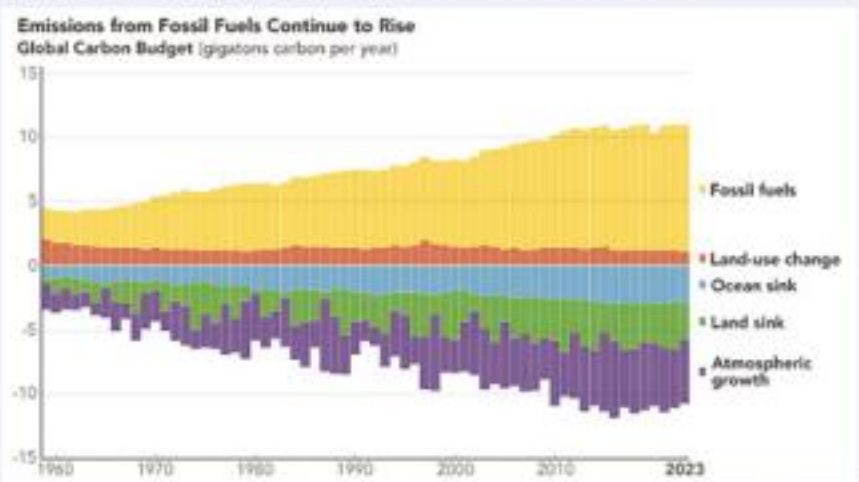


FIGURE 1 Global carbon budget (gigatons carbon per year).

General combustion reactions of fuels, shown below, are exothermic. In addition to heat, these reactions can produce carbon dioxide, carbon monoxide and water.

Complete combustion of fuels:

fuel + oxygen → carbon dioxide + water + heat

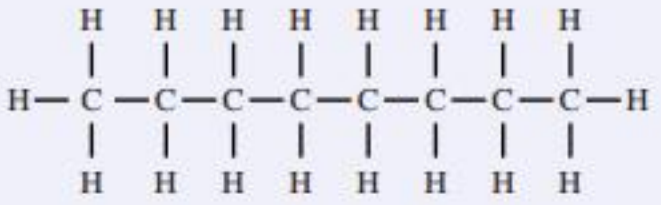
Incomplete combustion of fuels:

fuel + oxygen → carbon dioxide + carbon monoxide + water + heat

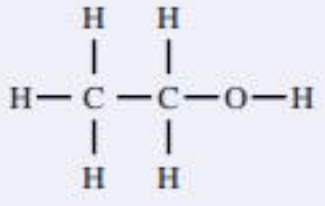
In the claim, efficiency in fuel usage encompasses a broad spectrum of terms, including complete and incomplete combustion and energy generation. Environmental impact could relate to gases produced during fuel combustion including CO_2 (Donev, 2024) or energy and resources used (production, transport and use) and possible land use/degradation.

Fossil fuels, such as oil, are formed from decomposition of plants and animals, deep within the Earth (National Geographic, 2024). Crude oil is distilled to a range of hydrocarbons that collectively make up fuels used in transportation. On the other hand, biofuels are renewable alternatives produced by fermenting sugars from sustainable sources like sugar cane (Queensland Government, 2024).

This study compares petrol (primarily octane) with ethanol; the structures of these compounds are shown in Figure 2.



Petrol (octane)



Ethanol

FIGURE 2 Structures of octane (found in petrol) and ethanol (bioethanol).

Petrol (gasoline) and bioethanol are examples of fossil fuels and biofuels, respectively, with ethanol already widely used as a 10% petrol additive (Wang et al., 2015) in Australia but higher proportions in fuels overseas. Due to the importance of replacing fossil fuels with biofuels, these two fuel types will be compared based on CO_2 emissions during combustion (see reactions below) and water used in their production.

The complete combustion equations for octane and ethanol:

octane: $2C_8H_{18}(l) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(g)$
$\Delta H = -5470\,kJ\,mol^{-1}$

ethanol: $C_2H_5OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(g)$
$\Delta H = -1360\,kJ\,mol^{-1}$

Research Question

Does bioethanol have less environmental impact, with regards to lower CO_2 emissions during combustion and lower water consumption during production and use, compared to petrol (octane)?

1.14 Analysing

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- identify the variables in the research question
- determine the evidence required to evaluate the validity of the research question
- identify relevant patterns and trends in the data
- explain the patterns between the two variables
- identify the limitations or gaps that exist in evidence.

The ISMG for the Analysing criterion, shown in Table 1.14.1, is assessed in relation to the identification of just enough data that enables the research question to be answered and identification of the limitations of the sources of the data.

TABLE 1.14.1 The performance characteristics associated with the highest performance level of the Analysing criterion.

Criteria	Assessment objectives	Performance Characteristics	Marks
Analysing	3. Analyse research data about the properties and structure of organic materials or chemical synthesis and design.	• the identification of sufficient and relevant evidence • thorough identification of relevant trends/patterns/relationships in evidence • thorough and appropriate identification of limitations of evidence	5

There are three aspects to the Analysing criterion.

To achieve the highest mark (5) in the Analysing criterion, you need to identify sufficient and relevant evidence to analyse the data and identify trends or patterns in the evidence. Finally, you need to identify the limitations of the evidence.

ANALYSING EVIDENCE

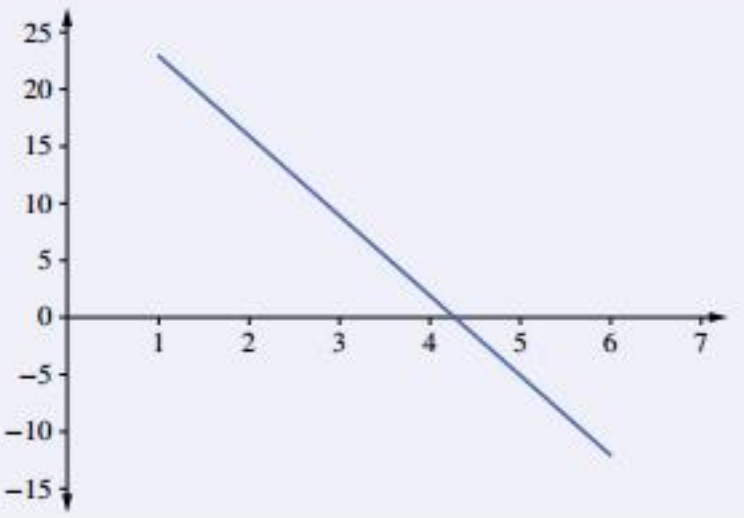
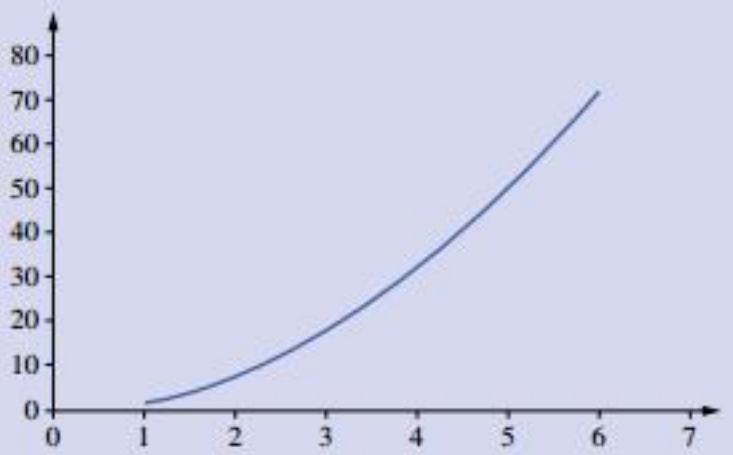
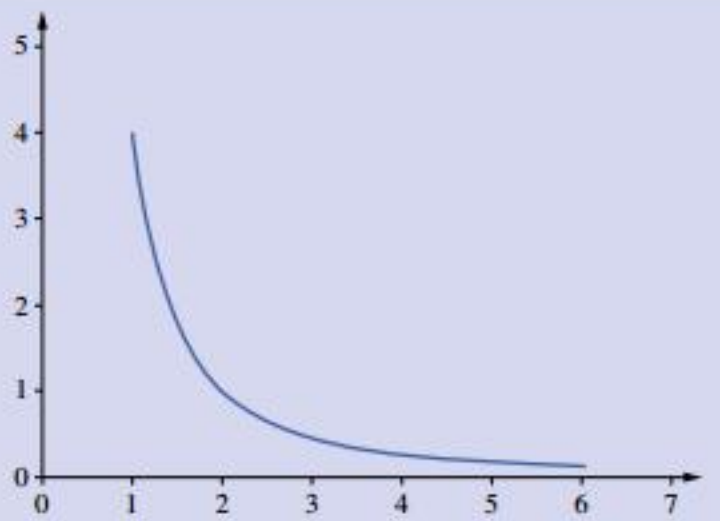
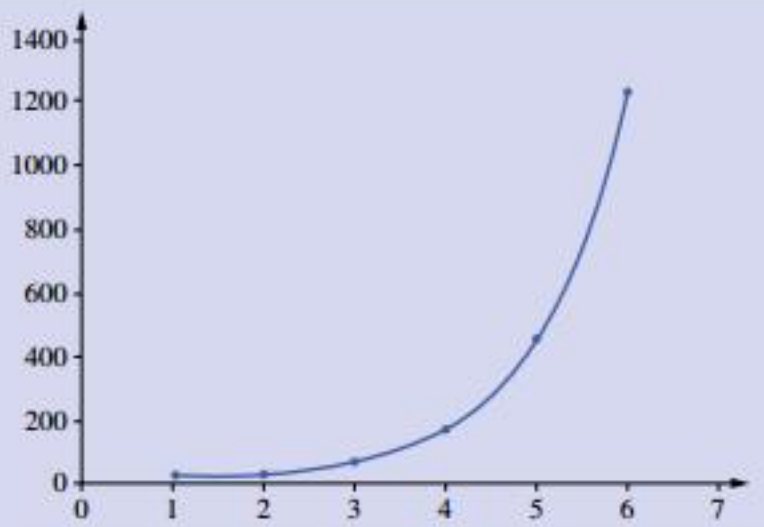
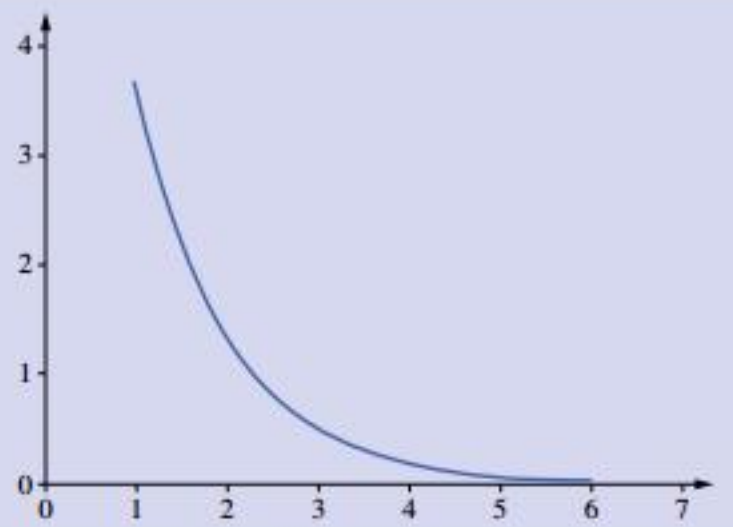
A trend or pattern is the general change in one characteristic with respect to another. In science, these are generally represented in the form of a graph with the dependent variable on the *y*-axis and the independent variable on the *x*-axis.

The first thing to notice about the trend is the shape of the graph. If there is a relationship between two variables, the trends can typically be categorised into one of five categories; linear, power, inverse, exponential and logarithmic.

In addition to the type of relationship, there are other factors to describe. For instance, does the dependent variable increase as the independent variable increases? Does the increase get bigger, as is the case with an exponential growth or does it plateau, consistent with a logarithmic change? Another way to describe a data set is by calculating the percentage difference. For example, when comparing the degree of biodegradability of two plastics over a 28-day period, this method can help quantify the relative differences. It is also important to consider that data may be presented from more than one source. The overall trend should be identified by comparing and synthesising findings from several authors to ensure a comprehensive understanding of the relationship.

Examples of the different shapes for graphical relationships are shown in Table 1.14.2.

TABLE 1.14.2 Examples of different graphical relationships: linear and non-linear (power, inverse, exponential, logarithmic)

Type of graph	Examples
Linear	
Power	 
Inverse	
Exponential	 

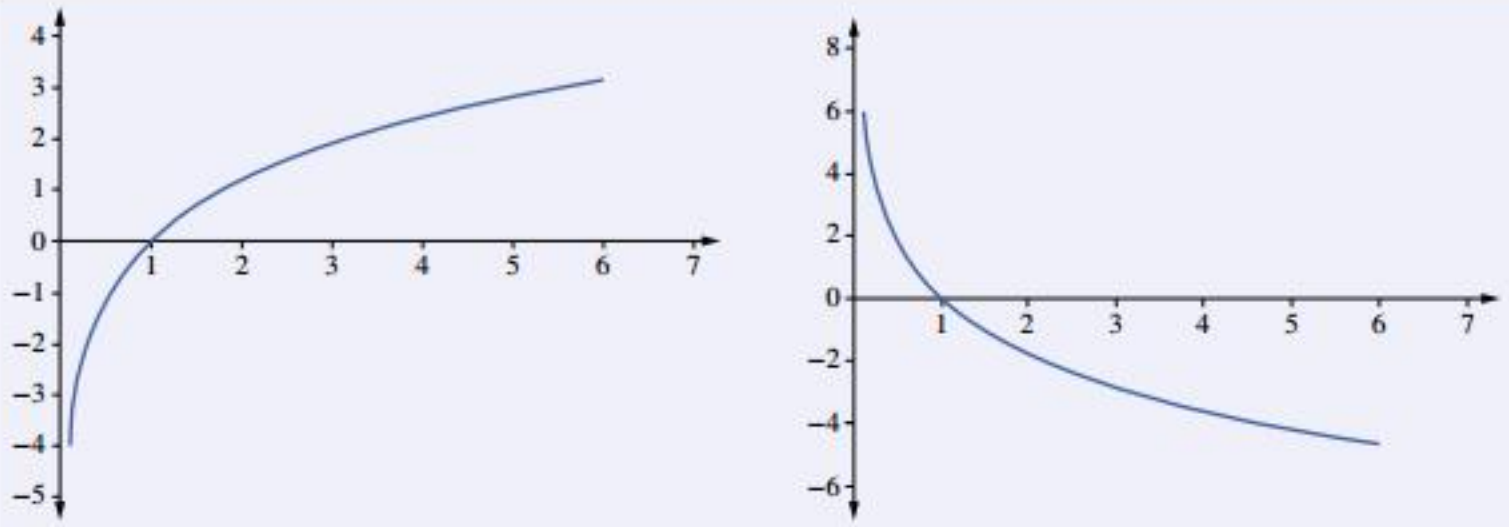
Type of graph	Examples
Logarithmic	

Figure 1.14.1 shows a comparison of two linear trends. The graph shows the change in the mass of product as a function of time. While a trendline for each is shown, no error bars are included for this discussion. When analysing relationships, it can be necessary to compare the effects of changing conditions on the dependent variable. In addition to determining the gradients of the curves, key features such as the *x*- and *y*-intercepts are important. While both linear graphs show that as time increases the mass of product increases, the rate of increase or gradient is greater for the dashed line. The dashed line passes through the origin, whilst the solid line extrapolates at a negative intercept.

Note that the analysis criterion requires you to identify the relationship but not the reasons for the relationship. That will be assessed in the Interpreting criterion.

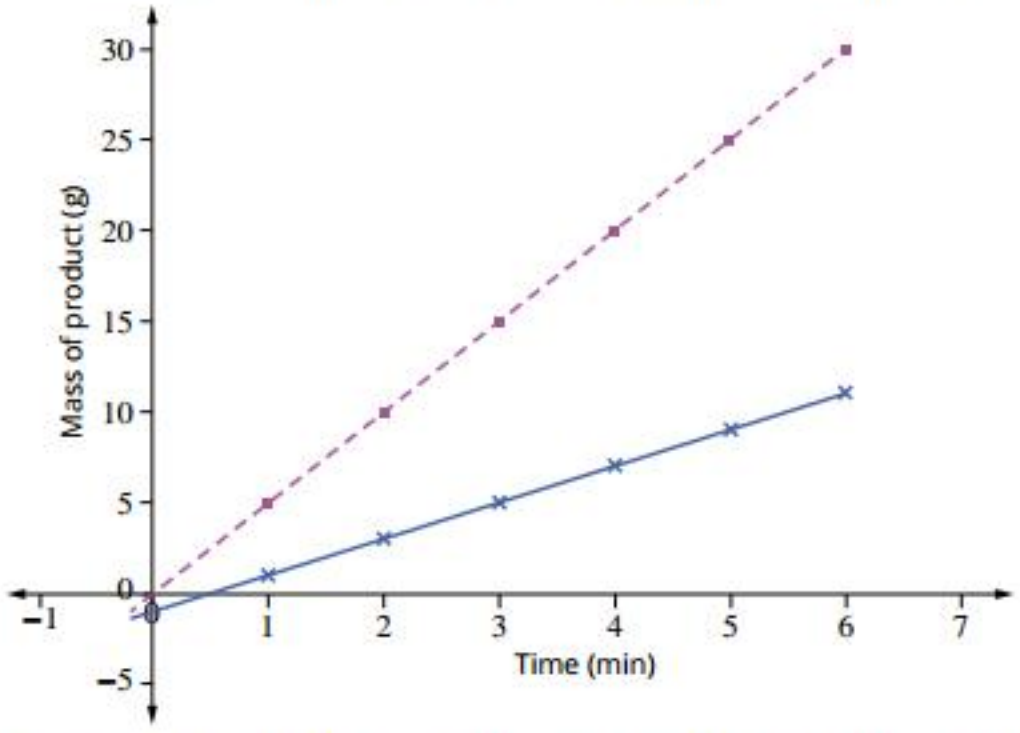


FIGURE 1.14.1 Comparison of the formation of product of a reaction under different conditions.

LIMITATIONS OF THE DATA

All studies are affected by limitations. So, when analysing the data, it is important to identify the limitations. Limitations can often be grouped into three categories:

- Elements of the methodology
- Study design that impacts the interpretation of the research results
- Differences between the studies or sources used to investigate the relationship

Examples of common methodological issues include:

- selection of samples

  Selection bias can occur if the sampling method results in the selection of samples that do not reflect the general population or population concerned.
- insufficient sample size for statistical measurements

  It is critical to have a sufficient sample size to draw valid conclusions. More precise results can be obtained if a larger number of samples are collected, which also enable the results to be generalised to a larger population. In contrast, if the sample size is too small, it can be difficult to identify significant relationships in the data.
- lack of previous research studies on the topic

  If the research cited is one of a limited number into the issue, the lack of available or reliable data can make it difficult to draw firm conclusions, or make connections between studies or the findings and the real world.
- methods/instruments/techniques used to collect the data

  While it is unlikely that the students will have experience in using many of the instruments used to collect the data, the limitations in the methodology should be outlined in the discussion section of the research paper. This could include, but is not limited to, the instruments' level of detection.

The differences between the studies or sources used to investigate the relationship represent a possible third category. While they may have the same dependent and independent variables, they are unlikely to have used exactly the same methods or materials. Additionally, even if studies elucidate the same relationship between variables, they may show differences in the degree or extent of the relationship. For example, biodiesel may be shown to have lower energy content than diesel, but different studies might use oils from various plant sources or test waste cooking oil as a fuel, which may affect the results.

When reading the research papers, refer to the collection of sufficient and relevant raw data in Part B on page e81. This will help evaluate the analysis of the data and identify limitations of the methodology.

As with identification of the trends and patterns, the analysis criterion only assesses the identification of the limitations of the research. The role these limitations played on the data collected and potential impact of the study, including the inability to generalise the research findings, will form part of the Evaluating criterion.

Furthermore, the report should discuss possible ways to overcome the limitations in future studies, such as alternative methodologies and ways to avoid issues.

Ways to discuss the limitations

When identifying the limitations of the study, there are ways to introduce the discussion on the limitations.

- Possible limitations of the study include …
- The first is the…The second limitation concerns the…
- The empirical results reported by … should be considered in the light of some limitations.
- This research is subject to several limitations.
- The primary limitation to the application of these results is…
- The design of the current study is subject to limitations.
- The major limitations in this study that could be addressed in future research are first, the study focused on …. Second …

Having data sources that have used different testing methods or materials can create limitations in the ability to answer the research question. For example, a catalyst shown to promote a reaction and increase yield might be studied under different reaction conditions or temperatures in different sources. Note that you will be using data from a number of sources to determine the overall trend, and it is unlikely that these researchers used exactly the same methods or materials.

SUFFICIENT AND RELEVANT

Similarly when deciding whether the sources are relevant or sufficient, refer to module 1.10. The analysis criterion uses the terms *sufficient* and *relevant*. However, in this case, the terms refer to the evidence. Was the data that was analysed 'enough' and 'connected with' the investigation to enable the research question to be fully answered?

PUTTING IT ALL TOGETHER

When writing the research report, it is important to evaluate the report against each criterion in the ISMG to assess the quality of the response. The analysis criterion is focused on the evidence that is collected and identifying and describing patterns or trends that are evident and connected to the research question. Therefore, it is critical that you identify the aspects of the research question that need to be answered. This will enable the search for and selection of information related to these aspects.

Once the evidence has been found, the trends need to be identified and used to answer the research question. Remember that the analysis criterion is only assessed against identification of the patterns and identifying the limitations of the research. So, to get the highest mark, the report needs to collect and analyse enough information to answer the research question.

The sample research investigation report that follows covers the ISMG criteria and may be used as a reference tool. Use this as a model for reference.

Analysing

CO_2 Emissions

Wang et al. (2015) used an engine to determine CO_2 emissions of ethanol/petrol fuel blends under different engine loads (engine temperature of 80°C and speed of 2000 rpm). The study compared three fuels: pure gasoline (E0), 10% ethanol with gasoline (E10) and 10% ethanol with gasoline and water (E10W).

Figure 3 shows both E10 fuels emit less CO_2 (about 5%) compared to pure gasoline (8%) at 5 Nm. When engine load increased to 60 Nm, all fuels had similar CO_2 emissions between 13% and 15%.

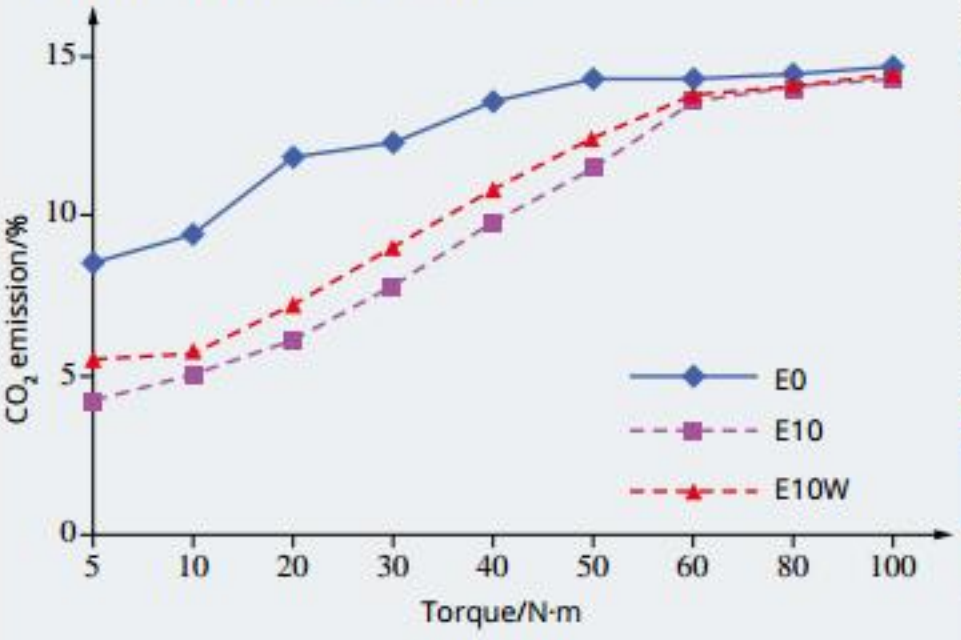


FIGURE 3 A comparison of CO_2 emissions for petrol blends at various loads.

The increases in emission for each fuel are relatively linear, although the gradient for pure gasoline is less, and plateau above 60 Nm.

This is consistent with tailpipe emissions reported by Natural Resources Canada (2014), which decreased from 2.29 to 1.61 kg L^{-1} as the percentage of ethanol increased.

Limitations

Wang's study (Wang et al, 2015) was conducted in the laboratory using a single engine type, with each test conducted only twice with the two results averaged. However, no information was provided about the variability of each measurement.

Values reported in the factsheet from Natural Resources Canada (2014) are estimates based on numerous factors from Environment Canada and report a single value despite emissions varying as a function of fuel density and composition.

TABLE 1 Comparison of CO_2 emissions of different fuels

Fuel	CO_2 tailpipe emissions (kg L^{-1})
Gasoline	2.29
E10 (10% ethanol/90% gasoline)	2.21
E85 (85% ethanol/15% gasoline)	1.61

Water use

Lampert et al. (2016) modelled water consumption associated with production, transport and use of various fuels. Figure 4 shows that gasoline has a much lower reliance on water than ethanol (166 L GJ^{-1} versus 1933 L GJ^{-1}, respectively) consistent with Wu et al. (2009) who showed that up to 6.6 L of water was required for each litre of gasoline produced compared to 324 L of water per L of ethanol produced.

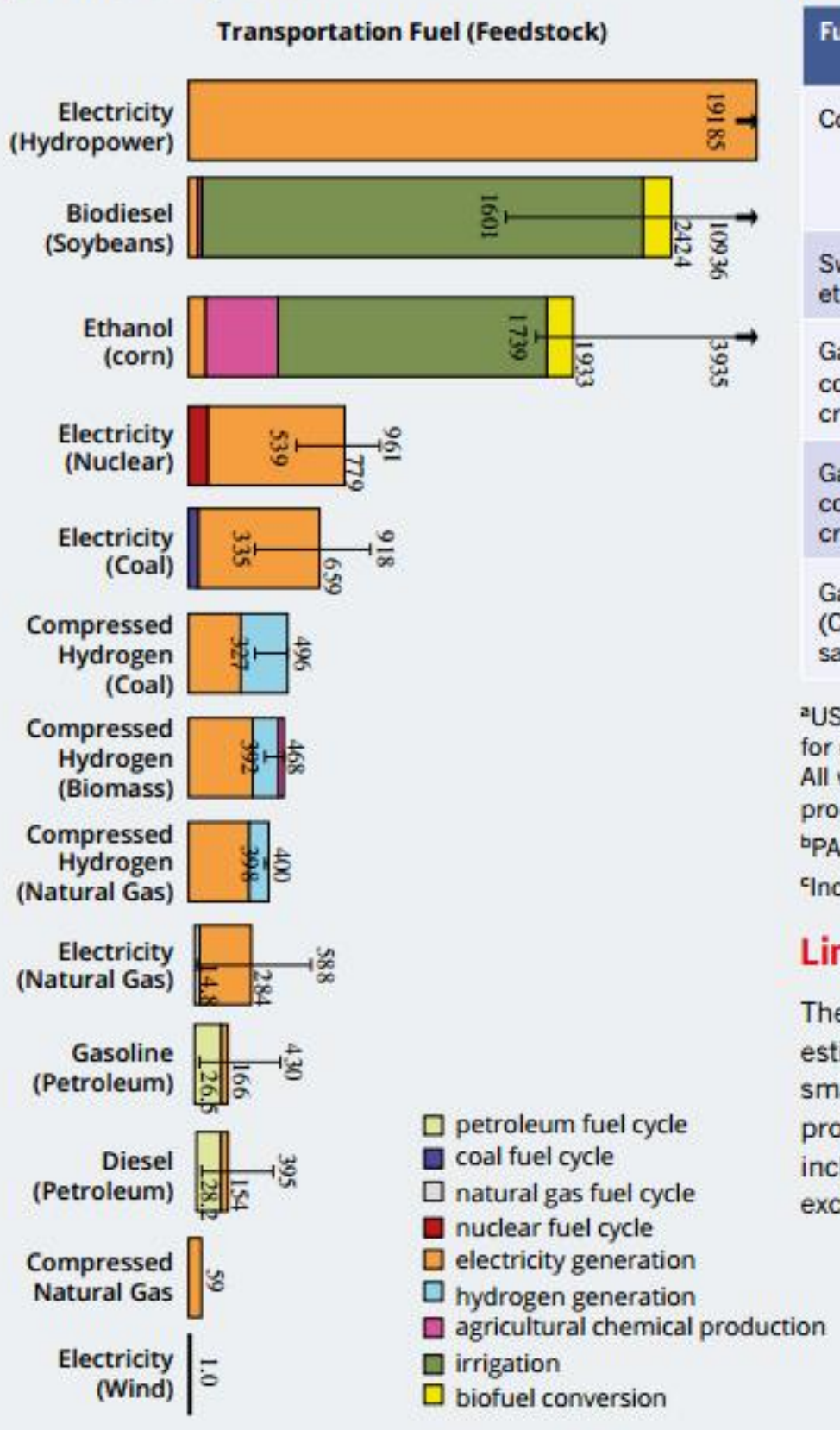


FIGURE 4 Water consumption (L per GJ) in production, transport and use of various fuels

Water used during fuel production (Table 2) included volume of water used for irrigation, excluding precipitation, and transportation. Corn ethanol has a large variation in water requirements, ranging from 10 to 324 L per L of ethanol due to regional variation in climate and soil compared with gasoline that has a water usage of 3.4 to 6.6 L/L gasoline.

TABLE 2 Water consumption in the production of ethanol and petroleum gasoline

Fuel (feedstock)	Net water consumed	Major factors affecting water use
Corn ethanol	10–324 L/L ethanol[a]	Regional variation caused by irrigation requirements due to climate and soil types
Switchgrass ethanol	1.9–9.8 L/L ethanol[a]	Production technology
Gasoline (U.S. conventional crude)[b]	3.4–6.6 L/L gasoline	Age of oil well, production technology, and degree of produced water recycle
Gasoline (Saudi conventional crude)	2.8–5.8 L/L gasoline	Same as above
Gasoline (Canadian oil sands)[c]	2.6–6.2 L/L gasoline	Geologic formation, production technology

[a]USDA regions 5, 6, and 7 combined for corn. Water consumption for corn, switchgrass, forest wood farming includes irrigation. All water used in ethanol conversion is allocated to the ethanol product

[b]PADD II, III, and V combined

[c]Including thermal recovery, upgrading, and refining

Limitations

The error bars (shown in Figure 4 and Table 2) in estimating water consumption in fossil fuel use are much smaller than those associated with natural sources as the production of crops is heavily dependent on many factors, including irrigation, soil type and natural rainfall, which is excluded from the study.

1.15 Interpreting

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- evaluate the research process
- understand the steps and requirements for a justified argument
- identify the steps necessary to develop a justifiable conclusion

The ISMG for the Interpreting criterion, shown in Table 1.15.1, is assessed in relation to creating scientific arguments and a conclusion and use of scientific language to address the research question.

TABLE 1.15.1 The performance characteristics associated with the highest performance level of the Interpreting criterion

Criteria	Assessment objectives	Performance Characteristics	Marks
Interpreting	1. Describe ideas and findings about the properties and structure of organic materials or chemical synthesis and design. 4. Interpret research evidence about the properties and structure of organic materials or chemical synthesis and design.	• justified scientific argument/s • justified conclusion linked to the research question • fluent and concise use of scientific language/ representations	5

There are three aspects to the Interpreting criterion.

To achieve the highest mark (5) in the Interpreting criterion, you need to create justified scientific arguments and a justified conclusion to answer the research question and present the results in the form of a scientific report using fluent language and representations.

JUSTIFYING AN ARGUMENT

When constructing a scientific argument, the claim, the evidence and the scientific reasoning need to be considered:

- The claim is what is known.
- The evidence is how this is known.
- The scientific reasoning is why the evidence supports or refutes the claim.

The QCAA glossary of cognitive verbs defines justify as 'to give reasons or evidence to support an answer, response or conclusion; show or prove how an argument, statement or conclusion is right or reasonable'

A scientific argument is a statement supported by multiple pieces of evidence that is measured or observed. The argument links the evidence and reasoning together with scientific facts and knowledge. It is important to recognise that the argument could either corroborate the claim or provide evidence that refutes the claim.

Therefore, the investigation needs to use the information and evidence collected from the research to answer the research question rather than simply opinions or beliefs that cannot be empirically verified.

The Introduction outlined terms and concepts related to the topic, which were used to develop the research question. This helped identify variables linked to the research question to be analysed. Then, the Analysis section of the report identified patterns and trends in the data related to the research topic.

The Interpretation section of the report needs to explain the trends between the variables to explain the research question.

Common things to avoid

When writing the justification, it is important to be concise and to the point. Select data and explain how the evidence is linked to the research question. Ignore evidence that has no relevance to the research question.

Be selective about the information discussed. The specifications of the assessment task state that the length of the report is limited to 2000 words. The justification needs to emphasise the significance of the research to the research question or topic. How do the trends identified in the Analysis section support the conclusion that was drawn? If the data does not directly address the question, it should be removed from the report. It is not necessary to use the whole of the data from the research; only use parts of the data that address the research question.

DRAWING A CONCLUSION

When writing the conclusion, make sure that it explicitly answers the research question. The easiest way to do this is to state the research question and summarise how the evidence supports the research question in about 150 words. In the summary, refer to the key evidence and authors or figures. In addition, concisely outline key limitations and how they contradict the conclusion with respect to the research question. The conclusion usually contains the scientific argument for the dependent and independent variable relationship that has been identified.

PUTTING IT ALL TOGETHER

There is no singular way of creating a justified argument to answer the research question or write the conclusion. The interpretation of the research collected simply needs to create justified arguments that use the evidence to explain and answer the research question to form a justified conclusion.

The sample research investigation report that follows covers the ISMG criteria and may be used as a reference tool. Use this as a model for reference for justified arguments that link the research question and evidence, enabling a conclusion supported by reasoning and scientific understanding to be drawn.

Interpreting

Data shows that octane generates more CO_2 per litre of fuel burned. When 1 mole of octane is burned, more energy is released compared to ethanol (NIST Chemistry Webbook), which is not surprising as octane forms more C=O and H–O bonds in carbon dioxide and water per mole.

TABLE 3 Comparison of thermodynamic data and moles of CO_2 produced as a function of energy and volume of fuel burned

Compound	Heat of combustion ($kJ\ mol^{-1}$)	Moles CO_2 produced ($mol\ kJ^{-1}$)	Moles CO_2 produced ($mol\ L^{-1}$)
ethanol	1366.3	1.46×10^{-3}	34.2
octane	5430	1.47×10^{-3}	49.2

Based on thermodynamics, CO_2 emissions for the fuels are almost identical. However, when density is taken into account, octane produces 43% more CO_2 per litre of fuel burned than ethanol (Table 3). This is consistent with observations of higher CO_2 emissions from gasoline than ethanol (Wu et al., 2016). However, since only 10% of the fuel was ethanol (E10 and E10W), this cannot account for the whole of the difference (8% compared to about 5%) at 5 Nm torque. The 43% higher emission for pure gasoline ($mol\ L^{-1}$) is of a similar magnitude to the estimate from Natural Resources Canada (2024), which reports that CO_2 emission with gasoline is about 42% higher than the 85% ethanol mix.

One limitation of this approach is that it does not take into consideration the engine efficiency, driving styles and engine age with respect to the fuels.

As engine torque increased, the difference in CO_2 emissions for the fuels decreased to become negligible above 60 N m, suggesting either a change in combustion efficiency of the engine at higher loads or that octane combustion is less complete so carbon monoxide is produced.

While emissions appear to be higher for gasoline, the greater energy stored in octane means that the two fuels produce similar amounts of CO_2 per kJ of energy produced, so would be as environmentally harmful as each other with respect to CO_2 release.

Interpreting *continued*

Lambert et al. (2016) and Wu et al. (2009) both show that bioethanol production consumes varying amounts of water from 1.9 L to 324 L of water per litre of ethanol (Table 2) due to varying irrigation requirements, whereas gasoline production uses significantly less water from 2.6 L to 6.6 L to produce the same amount of fuel. This is due to the different nature of the fuels and their production. Crop cultivation (biofuel) requires water, which if not provided by the rain is reliant on extensive irrigation. The locations of the corn farms (or sugar in Australia and Brazil) across US account for the large variability in the values in the studies as the growth of crops depends on the soil and water irrigation usage and would vary based on natural rainfall and irrigation from local water sources. Furthermore, biofuel production is a relatively new process that is less optimised and developed than the processing of crude oil, which is over 100 years old.

These two studies are limited in investigating water used in fuel production and do not take into account water use during other aspects. Additionally, the studies provide water use in different units, limiting comparison as ethanol and octane have different energy content (1366 kJ/mol and 5430 kJ/mol, respectively).

Conclusion

While 43% more carbon dioxide is emitted per litre for gasoline, when calibrated to the amount of energy generated both fuels produce similar emissions of CO_2 (1.46×10^3 mol kJ^{-1}). If engines for both fuels are equally efficient, then for the same distance travelled the same amount of carbon dioxide is produced. However, the production, transport and use of bioethanol requires more water as a result of irrigation required for the growth of the crops.

Therefore, the research question is disproven as while both fuels emit the same amount of carbon dioxide to travel the same distance, much more water is required in the production, transportation and use of bioethanol.

1.16 Evaluating

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- evaluate the research process
- identify the steps necessary to develop a justifiable conclusion
- evaluate the quality of the evidence
- extrapolate the conclusion to the original claim.

The ISMG for the evaluating criterion, shown in Table 1.16.1, is assessed in relation to evaluating the quality of the evidence, generalising the information to the original claim and suggesting improvements and extensions that relate to the claim.

TABLE 1.16.1 The performance characteristics associated with the highest performance level of the Evaluating criterion

Criteria	Assessment objectives	Performance characteristics	Marks
Evaluating	5. Evaluate research processes, claims and conclusions about the properties and structure of organic materials or chemical synthesis and design.	• justified discussion of the quality of evidence • extrapolation of credible findings of the research to the claim • suggested improvements and extensions to the investigation that are considered and relevant to the claim	5

To achieve the highest mark (5) in the Evaluating criterion, you need to evaluate the quality of information used to support the scientific arguments. This requires an explanation of the limitations of the data including an assessment of the statistical quality of the data, such as R^2 value or error bars. In addition, while the focus of the report is to justify a very narrow research question, this section needs to generalise the findings to the much wider claim, i.e. if the findings were more widely applicable, how would this impact the claim? Finally, identify improvements and extensions to strengthen the findings and further justify the answer to the research question.

EVALUATE THE QUALITY OF EVIDENCE

The analysis section of the report identified limitations in the data. This section of the report needs to explain how the limitations identified in the data and the sources used to support the argument affected the ability to evaluate and answer the research question.

Questions that could be useful to answer when evaluating the reliability of the data include:

- Were the statistical measures of the data good and appropriate?
  This could be shown by an R^2 value close to 1 or very small error bars in the data trend.
- Was the sample size sufficient to say that the findings were valid?
  As the sample size increases the standard deviation of the results decreases, meaning that the chance of results being skewed by a single outlier is less.
- Were the findings reproducible?
  The results of the research investigation were corroborated by other studies and research institutions.
  The experiments in the study were repeated with different techniques and the findings were consistent or independent of the methodology chosen, without a justifiable reason why they might vary.
- Did the result occur only under very specific conditions and were these conditions applicable to the real-world scenario?

- Was the methodology and instrumentation able to be applied appropriately to the situation studied?
- If the study had to investigate concentrations significantly greater than those that exist in the real world, can the findings of the research be applied to the real world?
- Are the theories that the authors used to support their findings still valid?
- Do the results fit the accepted theories or equations? For instance, in Figure 1.14.1, one of the trendlines went through the origin. This means that at the start of the experiment the mass of products formed was 0 g; however, the other trendline went through −1 g. This makes no sense in relation to the experimental data and so indicates that the results of this study may not be reliable. It is likely that these issues will have been identified and discussed by the authors in a peer-reviewed journal.

It is important not to just repeat the statements earlier in the analysis but to describe the effect on the investigation.

In addition to evaluating the data analysed, the investigation needs to evaluate whether the sources that were used were reliable.

EVALUATING SOURCES FOR VALIDITY AND RELIABILITY

Determining the validity and reliability of a source can be a challenging task. For some sources, it is easy to find details about the author, evidence and concurrency, while others only contain content and do not offer any other details. Another difficulty is when learning about a new topic or concept, we are all novice learners so it can be challenging to tell if a source is valid or not.

Examples of questions to consider when evaluating the sources include:

- Who or what organisation commissioned the report?
- What qualifications do the authors have?
- Is the source peer-reviewed or have a bias that might influence their findings?
- Is the information provided referenced and are the sources of this information reliable?
- When was the research reported? This is important as theories and concepts can be influenced by the year in which they were published.
- Are the findings reported in the publication supported by other sources? This will be found in the introduction, where the author identifies background information and gaps in the current understanding of the topic.

Table 1.16.2 outlines an example of evaluating a resource step-by-step, for the research article (Figure 1.16.1) that relates to silica aerogels.

Effect of silica aerogel on thermal insulation and acoustic absorption of geopolymer foam composites: The role of aerogel particle size

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ABSTRACT

Silica aerogel features super thermal insulating and excellent sound absorption. Although the application of silica aerogel in building materials for energy saving has been investigated recently, the role of aerogel particle size on geopolymer foam render can be crucial but is rarely studied. In this research, four kinds of silica aerogel with different particle sizes (2–40 μm, 100–700 μm, 100–1200 μm, 700–4000 μm) are applied in geopolymer foam aerogel render (GFAR) to improve the thermal insulation and acoustic absorption performance. Results show that larger silica aerogel particles are more beneficial for acoustic absorption and thermal insulation while smaller aerogel particles are less effective for insulation properties. The microstructure of GFAR is investigated in-depth with micro-CT, optical microscopy and ultrasonic pulse velocity test. The mechanism of the improved performance of GFAR with different silica aerogel is explained. The optimal geopolymer foam aerogel render (GFAR) reaches a thermal conductivity of 0.133 W/(m·K), an average value of acoustic absorption coefficient of 0.51 with a density of 715.2 kg/m^3. The result of this study is essential to enlighten the use of larger silica aerogel particles in geopolymer foam render, focusing on a low dosage of silica aerogel while utilize its full benefit.

1. Introduction

The energy-saving of the building sector and the comfort of the indoor living environment have received rising attention due to the increasing awareness of sustainability and the quality of life [1]. The building industry is responsible for almost 40% of the total energy and CO_2 emission in developed countries [2]. For now, many countries have already initiated policies to decrease heat loss through building shells [3]. Moreover, the functionalization of insulation materials is also very important, for instance, improving the acoustic absorption performance to increase the quietness of the indoor environment [4,5] and reduce the noise pollution generated from daily life [6]. Therefore, developing newly high-performance insulating lightweight materials is of significant urgency.

Silica aerogel is a super-insulating inorganic material [7], consisting of a 3D network of crosslinking silica nanoparticles and 95%–99% of air [8]. Thanks to the high porosity and low solid thermal conductivity (λ), the effective thermal conductivity of silica aerogel is pretty low, normally achieving 0.012–0.018 W/(m·K) [9]. However, the silica aerogel is very brittle and easy to break, the commercial silica aerogels are always produced in a powder or particle form [10]. It is often incorporated in other matrices, like fibreglass mats or other lightweight materials to facilitate its benefits [11]. Several investigations related to the incorporation of silica aerogel in building materials have already been carried out as presented in Table 1. Ng et al. [12] prepared high-performance aerogel concrete, with bulk density and thermal conductivity of 1300 kg/m^3 and 0.4–0.5 W/(m·K), respectively. The concrete has a low water to binder ratio of 0.20–0.25 and a silica aerogel replacement ratio of 50%–70% with sand. Tao et al. [13] developed normal cement mortar with an aerogel replacement ratio of 60%, featuring a compressive strength of 8.3 MPa and thermal conductivity of 0.26 W/(m·K). Júlio et al. [14] prepared lightweight aerogel aggregate concrete with a 100% replacement ratio of silica aerogel with sand, resulting in concrete with very low thermal conductivity of 0.085 W/(m·K) but compressive strength of only 0.41 MPa. Seo et al. [15] investigated the silica aerogel used in fly ash/slag geopolymer concrete, with an aerogel concentration of 25%–75%. However, the thermal conductivity is relatively high, reaching 0.8 W/(m·K). Zhu et al. [16] investigated the cement-based mortars and coatings with the addition of silica aerogel. The thermal conductivity is low (0.17 W/(m·K)) with a

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1359-8368/© 2022 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

FIGURE 1.16.1 A peer-reviewed research article entitled *Effect of silica aerogel on thermal insulation and acoustic absorption of geopolymer foam composites: The role of aerogel particle size.*

TABLE 1.16.2 Evaluation of a resource

Source evaluated: Effect of silica aerogel on thermal insulation and acoustic absorption of geopolymer foam composites: The role of aerogel particle size			
Criteria		**Decision**	**Support/justification**
primary or secondary	Is this an eyewitness account or a second-hand source?	primary	• Research article published in www.Sciencedirect.com • Research results published in article
validity	Does it contain information that is specifically related to the claim?	yes	• Outlines information directly related to the performance of aerogel as thermal insulation
	Is the evidence and information pertinent to the variables in the research question?	yes	• Information, experiment and results are specific to the performance and physiochemical properties of aerogel.
reliability	Is it current/recent information?	yes	• Published Aug 2022 • This is quite recent, but aerogels are modern materials undergoing a considerable amount of research. There may be newer information available.
	Is it up-to-date in its understanding of relationships?	yes	• Information outlined about thermal conductivity and properties of aerogel
	Is the evidence equivalent to other sources?	mostly	• Table 1 within the article contains a list of six similar experiments.
	Check the credibility—consider who the author is, their qualifications and expertise.	good	• Authors are from the School of Civil Engineering at Wuhan University or the Department of the Built Environment at Eindhoven University. • *Journal of Basic and Applied Sciences* is a reputable peer-reviewed journal
	Try to find the sample size.	known	• Six samples, three trials per sample.
	Try to establish what variables were controlled or measured.	known	• Methodology of the preparation, storage, and testing of the samples is detailed, including controlled variables such as air temperature and humidity

A judgement could be made about the credibility of this source, such as: "The information and evidence was published by experts in a peer-reviewed journal article that is concurrent and with variables of experimentation known and directly related to the claim and research question. However, as the results are new, it is yet to be seen if they are substantiated, therefore affecting the reliability of the evidence. This resource is both valid and reliable."

EXTRAPOLATION TO THE CLAIM

The first stage of this assessment involved narrowing the claim to a very specific research question. This could have meant selecting a specific material or smaller temperature or concentration range. The Extrapolating criterion requires inferring how the trends and patterns identified and explained in the earlier sections of the research report could be extended to the original claim.

When exploring the claim, the students identified the dependent and independent variables associated with the claim. Thus, questions that can help students extrapolate the findings and conclusion to the claim include:

- what are the dependent, independent and controlled variables associated with the claim?
- what is the impact on the dependent variable when the independent or controlled variables from the research question are extended to include the claim?

IMPROVEMENTS AND EXTENSIONS

Suggest improvements and extension(s) that would complement the research findings and have the potential to provide new evidence that could be used to evaluate the research question (improvements) and claim (extensions) further. These should be linked to the identified limitations (analysis and quality of evidence—make sure not to repeat yourself—can just identify the issue).

The highest performance level requires that suggested improvements need to be considered and relevant. There are two obvious areas that could be the focus of the suggested improvements. First, a good place to start when proposing possible improvements is the limitations in the research and evidence that were identified and explored in the previous sections in the report. Second, identify what information is required to provide more definitive proof of the research question.

As discussed in the limitations, these could come from the methodology or the interpretation of the results. It could be useful to consider the following:

- changes to the method of selecting samples to reduce bias
- increasing the sample size to increase the accuracy of the results or reduce the errors associated with the measurements
- methods/instruments/techniques used to collect the data. Were the measurements below the limit of detection or so low that the associated error was large? Has technology advanced since the previous research which means that the relationship can be more accurately determined?
- gaps in the evidence that you identified through your investigation.

These considerations could form the basis for your suggested improvements. While a detailed explanation of these is not required, the report should identify how they would benefit your investigation.

Suggestions of possible extensions to the research investigation could be identified from the information collected as part of the research investigation. Students should ask themselves if there were limits to the scope of evidence available.

- During the research, did you identify areas that could be explored further?
- Could the conclusions from your report be extended to another situation?
- When extrapolating the research question to the claim, were there any aspects that could not be proven because information was not available?

PUTTING IT ALL TOETHER

The sample research investigation report that follows covers the ISMG criteria and may be used as a reference tool. Use this as a model for reference.

Evaluating

Extrapolation to claim

While the research question is disproven, biofuels may be more efficient and have less environmental impact than fossil fuels as stated in the claim as these studies investigated only a few aspects related to environmental impact. The combustion of bioethanol releases the same amount of carbon dioxide to produce the same energy as gasoline; however, other environmental impacts such as biodegradability, land use and energy required during production have not been addressed. The efficiency (e.g. energy content) of biofuels and fossil fuels has not been investigated here and only one biofuel and fossil fuel are investigated. As not all aspects of environmental impact nor efficiency have been researched, the claim cannot be proven.

Quality of evidence

Studies (Wang, Chen, Ni, Liu & Zhou, 2015 and National Resources Canada, 2014) investigated the CO_2 emissions of ethanol compared to gasoline. However, Wang (2015) only investigated engine load parameter, which affects CO_2 emissions. If the load of an average passenger vehicle or transport vehicle is 60–100 Nm, the difference in CO_2 production per L during combustion is negligible (Figure 3) but as a function of energy, CO_2 production is less. This limits the ability to answer the research question and claim.

Wu et al. (2009) and Lampert et al. (2016) both model water use. However, units are different—L/L or L/GJ. This is a limitation because ethanol and octane have very different energy content, 1367 kJ mol^{-1} and 5430 kJ mol^{-1}, respectively. Water use of ethanol estimated per litre will need to be multiplied by approximately 4 to estimate water use to provide the same energy as gasoline.

Furthermore, the ability to conclude from Wu et al. (2009) is limited as the source is over 10 years old and may not be relevant to current water consumptions of ethanol and petrol. However, all sources are retrieved from peer-reviewed scientific journals indicating their reliability. Also, the National Resources Canada data is limited and uses second-hand modelling data.

Improvements and extensions

To fully determine the environmental impact of bioethanol with respect to CO_2 emissions and water consumption during production compared to petrol, further testing is required. Further studies on the production, transport and use for each fuel are required as only one author is provided.

The use of water showing bioethanol is a greater risk to the environment is complicated by the fact that technologies for ethanol production are not optimised as with crude oil and petrol which is over 100 years old. Information is required about more up-to-date biofuel production techniques which likely are more efficient. This means negative environmental effects of producing bioethanol may decrease and feasibility of using the fuel will increase.

More information relating to the general engine loads of vehicles using these fuels is required and carbon dioxide emitted as a function of distance travelled.

To further answer the claim, the efficiency of a larger range of biofuels compared to fossil fuels should be investigated, such as biodiesel and biogas. Furthermore, the efficiency of more engines should be investigated as Wu et al. (2015) only investigated one engine. Environmental impact can be further investigated by analysing energy related to the production and use of alternate fuels.

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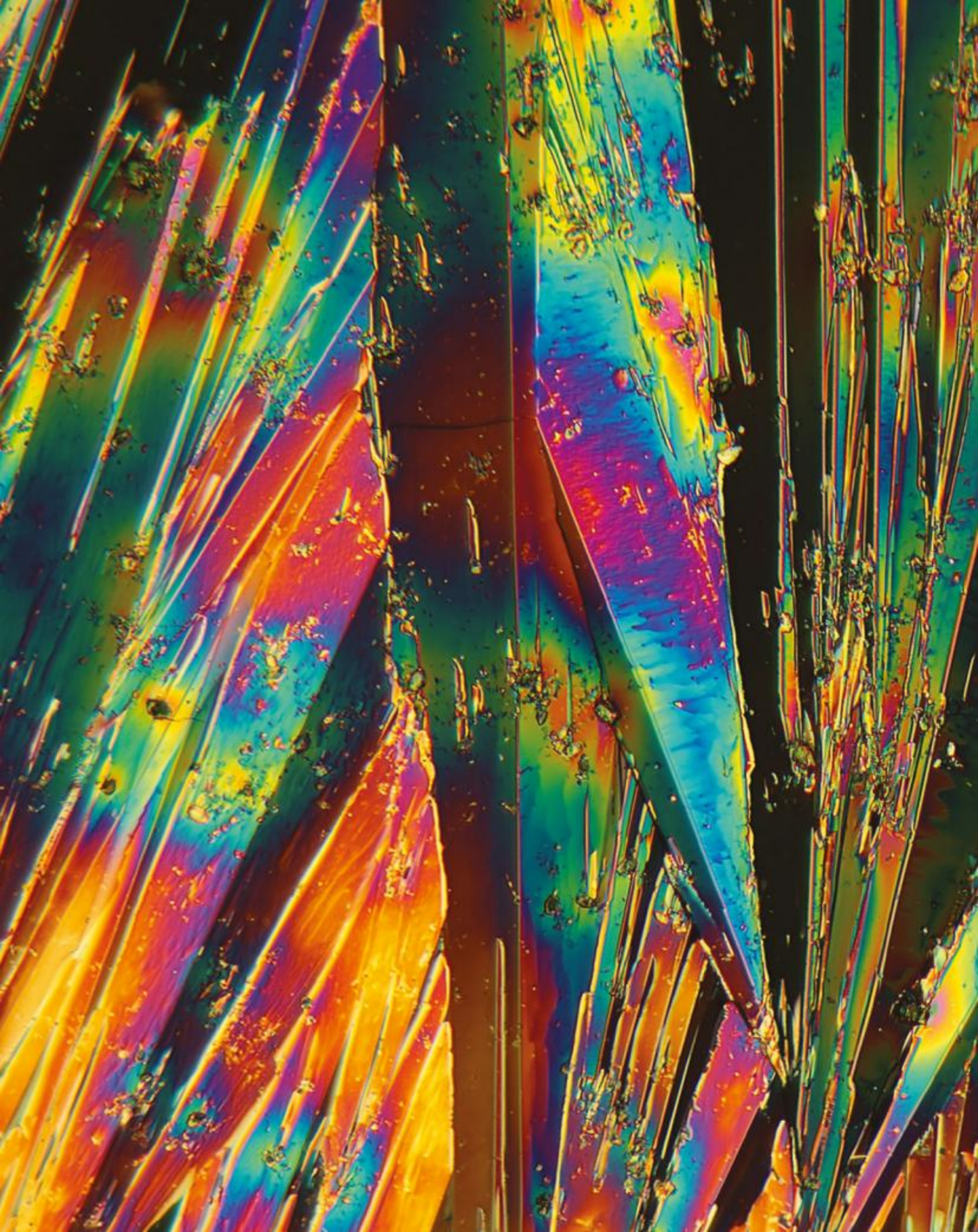
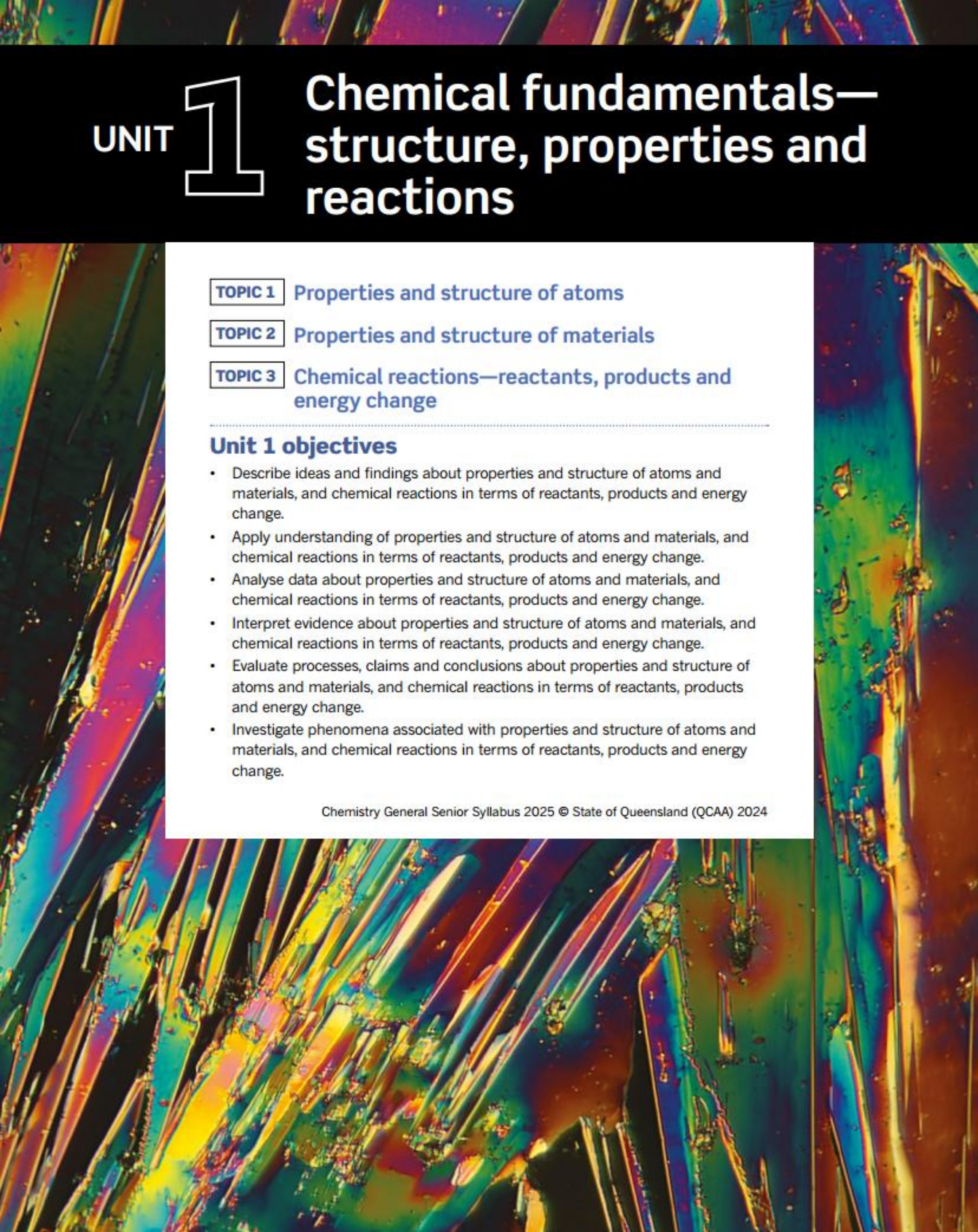


UNIT 1 Chemical fundamentals—structure, properties and reactions



TOPIC 1 Properties and structure of atoms

TOPIC 2 Properties and structure of materials

TOPIC 3 Chemical reactions—reactants, products and energy change

Unit 1 objectives

- Describe ideas and findings about properties and structure of atoms and materials, and chemical reactions in terms of reactants, products and energy change.
- Apply understanding of properties and structure of atoms and materials, and chemical reactions in terms of reactants, products and energy change.
- Analyse data about properties and structure of atoms and materials, and chemical reactions in terms of reactants, products and energy change.
- Interpret evidence about properties and structure of atoms and materials, and chemical reactions in terms of reactants, products and energy change.
- Evaluate processes, claims and conclusions about properties and structure of atoms and materials, and chemical reactions in terms of reactants, products and energy change.
- Investigate phenomena associated with properties and structure of atoms and materials, and chemical reactions in terms of reactants, products and energy change.

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CHAPTER

02 Elements, compounds and mixtures

Chemistry is the study of matter: its properties, composition and transformations; how certain types of matter interact with other types of matter; and how matter interacts with energy such as heat, visible light and ultraviolet radiation. In this chapter, you will learn what matter is, the different types of matter that exist and how matter changes from one type to another. You will also recognise that most matter actually exists in impure forms as mixtures of pure substances (elements and compounds) and that these mixtures can take the form of homogeneous mixtures or heterogeneous mixtures.

Syllabus subject matter

Topic 2 • Properties and structure of materials

■ COMPOUNDS AND MIXTURES

- State that pure substances may be elements or compounds. **2.1**
- Identify that pure substances have distinct measurable properties (e.g. melting and boiling point, reactivity, strength, density) and mixtures have properties dependent on the identity and relative amounts of the substances that make them up. **2.1**
- Discriminate between heterogeneous and homogeneous mixtures. **2.2**
- Analyse data to determine the physical properties of pure substances and mixtures. **2.1**

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2.1 Characterising matter

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that matter can be characterised by its purity
- understand that most matter you encounter in your everyday life is a mixture of pure substances
- recall that mixtures may be homogeneous or heterogeneous
- recognise that mixtures are materials where the properties are dependent on the identity and relative amounts of the substances that make up the mixture
- state that pure substances are either elements or compounds
- identify that pure substances have a definite and distinct set of physical and chemical properties.

Chemistry is the study of **matter**, so it is important to understand the different types of matter that exist. You know from everyday experience that a tree, a rock, a glass of water and a piece of gold are examples of matter. You also intuitively know that there are fundamental differences in the observable properties of trees, rocks, water and gold that tell us that they are different types of matter. However, you can identify some properties common to all types of matter. For example, you can see the effect of matter on other matter; think of the book you are reading or the screen you are viewing; think of the wind on your face, the sand between your toes or the water in your bathtub. All are examples of matter.

Another characteristic feature of matter is that you can measure it. Matter has **mass** and you can measure this **physical property**; matter also occupies space and you can measure its **volume**. The following statement is a good working definition of matter that will suit our purposes for studying chemistry.

Matter can be described as anything that has mass, occupies space and can be perceived by our senses.

PURITY OF MATTER

Matter can be classified, or characterised, in different ways. One way is to look at the purity of matter. It turns out that most of the matter you encounter in your everyday life—including the food you eat, the air you breathe and the water you swim in—is not chemically pure. Most matter actually consists of **mixtures** of **pure substances**. For example, the air you breathe is a mixture of oxygen and nitrogen with trace amounts of other gases, including carbon dioxide, water vapour and argon. Even tap water may appear to be pure, but it actually contains trace amounts of dissolved minerals.

The relationship between pure substances and mixtures is shown in Figure 2.1.1. It shows that the matter you observe in your everyday life is ultimately composed of either elements or compounds. **Elements** contain only one type of **atom**, for example, oxygen (O_2) or carbon (C). **Compounds** contain two or more elements chemically bonded together, for example, carbon dioxide (CO_2) or sodium chloride (NaCl). Collectively, elements and compounds are known as pure substances. Pure substances can be physically combined to produce mixtures. Mixtures can either be homogeneous or heterogeneous. **Homogeneous mixtures** are uniform throughout, while **heterogeneous mixtures** are not uniform. The differences between these two types of mixtures will be discussed in detail in Module 2.2 of this chapter.

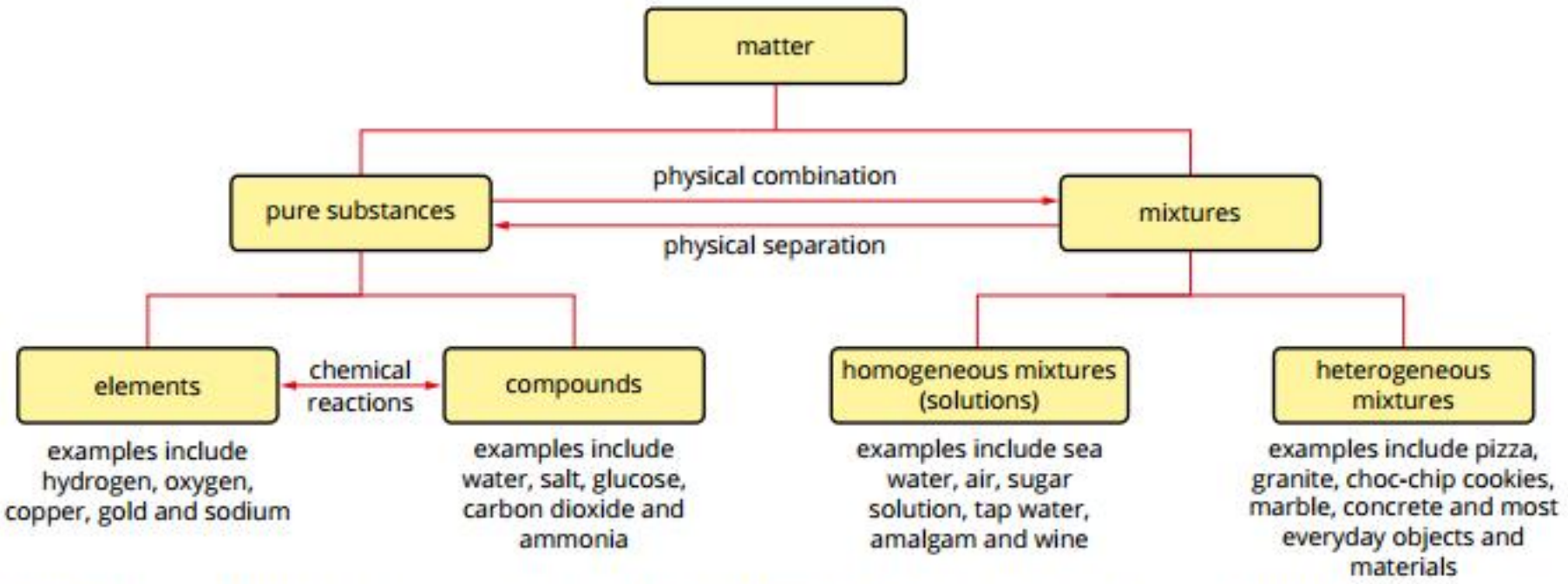

matter
physical combination
pure substances
mixtures
physical separation
elements
chemical reactions
compounds
homogeneous mixtures (solutions)
heterogeneous mixtures
examples include hydrogen, oxygen, copper, gold and sodium
examples include water, salt, glucose, carbon dioxide and ammonia
examples include sea water, air, sugar solution, tap water, amalgam and wine
examples include pizza, granite, choc-chip cookies, marble, concrete and most everyday objects and materials

FIGURE 2.1.1 Classification of matter according to purity, showing the relationship between elements, compounds and mixtures

Figure 2.1.2 shows four examples of different types of matter.

- A slice of pizza (Figure 2.1.2a) contains a mixture of carbohydrates, fats and oils, as well as water and dissolved minerals and nutrients. It is a physical mixture of a wide range of pure substances. It also contains visibly distinct 'chunks' that are different from other parts, such as the pepperoni slices. This indicates that a slice of pizza is a heterogeneous mixture.
- Food colouring dissolved in water (Figure 2.1.2b) is also a physical combination of two or more pure substances and is, therefore, a mixture. In this case, however, there are no distinct 'chunks' of matter that are visibly different from the rest of the coloured solution. The homogeneous nature of a solution of food colouring indicates that it is a homogeneous mixture. Many homogeneous mixtures are also known as solutions.
- The salt crystal (Figure 2.1.2c) is a pure substance and is not a physical combination of different substances. It is the compound sodium chloride (NaCl) and consists of elements chemically combined in a fixed ratio (i.e. sodium and chlorine in a 1:1 ratio).
- The sample of copper wire (Figure 2.1.2d) is also a pure substance and is an example of an element.

FIGURE 2.1.2 Examples of different types of matter: (a) a slice of pizza (heterogeneous mixture), (b) food colouring dissolved in water (homogeneous mixture; also a solution), (c) a salt crystal, which is a pure substance composed of the compound sodium chloride (NaCl) and (d) copper metal, which is an example of an element.

PHYSICAL AND CHEMICAL CHANGES IN MATTER

In chemistry, you need to understand how matter can change from one form to another. A change in the form of matter can occur via physical and/or chemical changes. Figure 2.1.1 shows that combining pure substances to create mixtures requires a physical change.

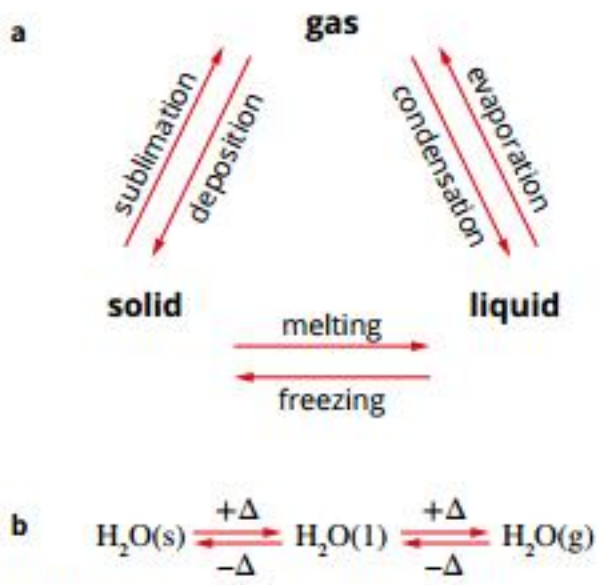


FIGURE 2.1.3 (a) Processes describing the changes of state between solids, liquids and gases. (b) The melting, boiling, condensing and freezing of water can be represented using chemical formulas and chemical equations. The bracketed letters, (s), (l) and (g), represent the solid, liquid and gaseous states of water. The '+Δ' and '−Δ' symbols refer to the need for 'energy required' or 'energy released' to induce the changes of state indicated.

Separating mixtures into their pure components also requires a physical change. Figure 2.1.1 further shows that to create compounds or to decompose them into their elemental components requires a chemical change or chemical reaction.

Physical changes in matter

A **physical change** in matter is a process where the form of matter may be changed without changing its chemical identity or its chemical composition. No new substances are formed during physical changes. Cutting a piece of paper, grinding a tablet and bending an iron bar are examples of physical changes.

A change in **physical state** is one of the most important types of physical changes. The melting of ice to produce liquid water or the heating of water to produce water vapour are examples of physical changes of state. No new substances are formed in changes of state. The processes involved in changes of state are summarised in Figure 2.1.3a and represented using chemical equations in Figure 2.1.3b.

Chemical changes in matter

Chemical changes in matter (i.e. chemical reactions) involve a change in chemical composition where one or more kinds of matter are transformed into a new kind of matter (or several new kinds of matter). In other words, **chemical reactions** involve the production of new substances. You can see the results of chemical reactions around you every day. The burning of wood, the spoiling of milk, the digestion of food and the growth of plants via photosynthesis are all examples of chemical reactions.

In simple terms, a chemical reaction can be described as a rearrangement of atoms. The combustion of hydrogen (H_2) in the presence of oxygen (O_2) to produce water (H_2O) is one of the simplest chemical reactions. It can be represented using the balanced **chemical equation** below:

$$2H_2(g) + O_2(g) \xrightarrow{\text{heat}} 2H_2O(l)$$

Here two elements, hydrogen (H_2) and oxygen (O_2), chemically combine to produce the compound water (H_2O). The equation is balanced, so the four hydrogen atoms and two oxygen atoms on the left-hand side of the equation are rearranged and incorporated into the two water **molecules** on the right-hand side of the equation.

MIXTURES

As Figure 2.1.1 on page 5 suggests, a mixture is a physical combination of two or more pure substances. This means there can be mixtures of:

- two or more elements (such as sterling silver—a mix of silver and copper)
- two or more compounds (such as salt water)
- elements and compounds (such as oxygen dissolved in water).

Figure 2.1.1 also suggests that mixtures such as these can be physically separated into their pure components by simple physical processes. Processes such as cutting, crushing, sieving, filtration, distillation or centrifugation can isolate pure substances from complex mixtures. The ability to separate mixtures into their pure components is crucial in many industrial, environmental and biomedical applications.

Mixtures can vary in composition from sample to sample with different types and amounts of substances being present. Since the composition of mixtures can vary, it follows that the chemical and physical properties of mixtures can also vary depending on the type and amount of substances present.

Figure 2.1.4 shows how the **boiling point** and **freezing point** of water change with small additions of sodium chloride (NaCl). The boiling point of pure water is 100°C and the freezing point is 0°C. Both change when other substances are mixed with water. The increase in boiling point is known as **boiling point elevation**. The more salt dissolved, the greater the change in boiling point. Likewise, the decrease in freezing point is known as **freezing point depression** and, again, the more salt dissolved, the greater the change in freezing point.

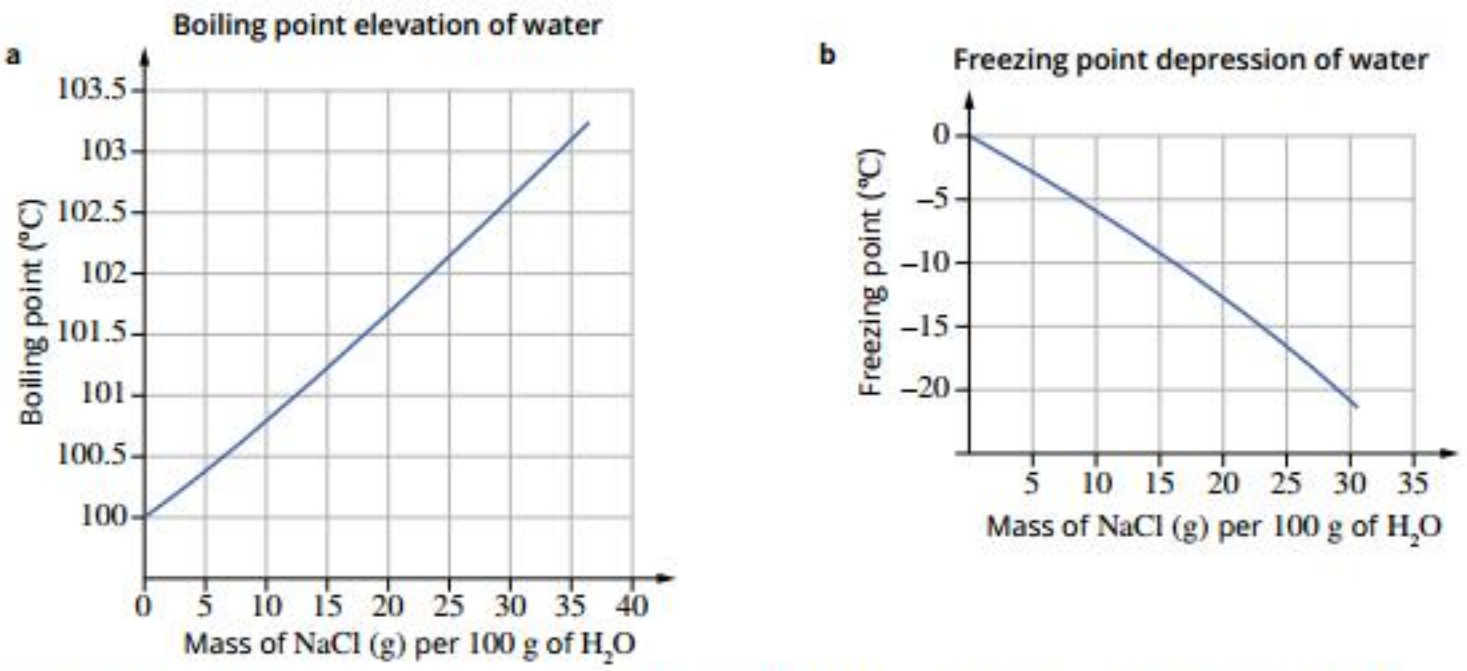


FIGURE 2.1.4 (a) Boiling point elevation—the boiling point of water increases with increasing amounts of NaCl. (b) Freezing point depression—the freezing point of water decreases with increasing amounts of NaCl.

Changes in physical and chemical properties, such as those shown in Figure 2.1.4, are useful for distinguishing between mixtures and pure substances. Mixtures have different physical and chemical properties depending on the type and amount of substances present. Pure substances, on the other hand, do not vary in composition and, therefore, do not vary in chemical or physical properties. Some of the chemical and physical properties that can be used when characterising different types of matter are shown in Table 2.1.1.

TABLE 2.1.1 Examples of chemical and physical properties that can be used to characterise different types of matter. These properties can be used to distinguish mixtures from pure substances.

Chemical properties	Physical properties
combustibility/flammability	freezing point
reactivity in water	melting point
reactivity with acids	colour
reactivity with bases	viscosity
oxidisability	density
pH (specifically changes in pH)	solubility
toxicity	electrical conductivity
radioactivity	thermal conductivity
decomposition with heat	malleability/ductility/hardness/strength

Mixtures of metals are called **alloys**. An alloy might have more useful properties than the metals it is made of. An example is the 18-karat gold used in jewellery. The purity of gold is measured in karats (kt). When it is 99.9% pure (24-karat), gold has only moderate strength and hardness and scratches easily. 18-karat gold is 75% gold and has greater strength, so it makes more durable jewellery. Sporting medals do not require the same physical strength as jewellery and are often made in 24-karat gold. This gives the medal some softness. Figure 2.1.5 shows an athlete proudly 'testing' the softness of her medal.

FIGURE 2.1.5 An athlete bites her gold medal to test its softness.

Many plastics are carefully designed mixtures of large molecules with specific physical properties. They are generally lightweight, durable, versatile, chemically resistant and quite cheap to produce. However, those plastics that are not biodegradable or recyclable can be an environmental problem.

Each type of plastic has particular uses, as outlined in Figure 2.1.6. Two key examples, which you will study in Unit 4, are high-density polyethene (HDPE, recycle number 2) and low-density polyethene (LDPE, recycle number 4). For low-density polyethene, the decrease in density results in greater flexibility but a decrease in strength.

Polyethene terephthalate	High-density polyethene	Polyvinyl chloride	Low-density polyethene	Polypropene	Polystyrene	Includes polycarbonates, ABS, Teflon, various copolymers, nylon and other condensation polymers
Bottles for soft drinks, water, shampoo, takeaway food containers	Garbage bins, fuel tanks, hard hats, banners, water pipes, food-storage containers	Plastic wrap, cordial bottles, electrical wire covers, water pipes, floor tiles	Plastic wrap, squeeze bottles, plastic tubing, shopping bags	Rope, clothing, ice-cream containers, flip-top bottle lids	Yoghurt containers, fridge shelves, drink cups, insulating beads, packaging	

FIGURE 2.1.6 An international number code is used to identify each type of recyclable plastic.

PURE SUBSTANCES

A pure substance (or simply a substance) is a matter that has a definite and distinct set of physical and chemical properties that do not vary in composition from sample to sample. In general, any two samples of matter that have identical chemical and physical properties are said to be the same substance. Therefore, chemical and physical properties (such as those outlined in Table 2.1.1 on page 7) can be used to identify a particular sample of matter. For example, a shiny, silver-coloured metal that has a melting point of 660.3°C, a **density** of 2.70 g cm^{-3} and reacts with acid to produce hydrogen gas (H_2) can only be the element aluminium (Al). This is because only aluminium has this definite and distinct set of chemical and physical properties.

There are two types of pure substances: elements and compounds. As Figure 2.1.1 on page 5 shows, elements combine by chemical reactions to form compounds, while compounds can be decomposed into elements by chemical reactions. Unlike mixtures, substances cannot be separated into other kinds of matter by simple physical processes such as filtration, distillation and centrifugation.

ELEMENTS

Elements are the simplest form of matter that exists. They cannot be broken down into other substances by simple physical processes, nor can they be broken down into other substances by chemical reactions. Elements are the building blocks of matter since they can combine chemically to form millions of different compounds. The defining feature of elements is that they are substances that contain only one type of atom. The monatomic gases helium (He), neon (Ne) and argon (Ar) are examples of elements; the diatomic molecules oxygen (O_2), nitrogen (N_2), hydrogen (H_2) and bromine (Br_2) are also examples of elements; so too are the metals sodium (Na), copper (Cu), aluminium (Al) and iron (Fe).

i Monatomic elements are those made up of only one atom. Diatomic elements are comprised of two atoms. The prefixes *mon* (or *mono*) and *di* are frequently used in chemistry. They mean 'one' and 'two', respectively.

Most non-metallic elements form molecules with a definite number of atoms. Sulfur, for example, is composed of molecules with eight sulfur atoms (S_8). However, some non-metals form **covalent network lattices** or **giant covalent networks**. Carbon is an example of such a non-metallic element. Diamond and graphite are both examples of covalent network lattices formed by carbon. Graphene is a giant covalent network formed by carbon. (You will learn more about covalent network lattices formed from carbon in Chapter 8.) Representations of the sulfur molecule and a carbon covalent network lattice are shown in Figure 2.1.7. Metallic elements form a different type of network lattice structure, which you will look at in detail in Chapter 6.

A molecule is a definite and discrete group of atoms chemically bonded together. The atoms in molecules are non-metallic atoms bonded to other non-metallic atoms.

Element names, symbols and numbers

At present, there are 118 known elements, 92 of them naturally occurring, while the other 26 have been synthesised in laboratories and are very unstable. Each element is assigned a unique name and **chemical symbol**. Chemical symbols are typically either a single capital letter (e.g. H for hydrogen) or a single capital letter followed by a lower-case letter (e.g. Ne for neon). Most chemical symbols make sense from their names (e.g. C for carbon or Mg for magnesium). Other symbols make less sense as their symbol may be derived from their Latin name (e.g. Au for gold, from the Latin *aurum*, or K for potassium, from the Latin *kalium*). Table 2.1.2 shows an alphabetical listing of some common elements along with their chemical symbols and some observable physical properties.

TABLE 2.1.2 Alphabetical listing of common elements including names (Latin name in brackets), symbols and some physical properties

Element	Chemical symbol	Physical properties
aluminium	Al	silvery metal
barium	Ba	silvery metal
bromine	Br	reddish liquid
calcium	Ca	silvery metal
carbon	C	soft, black solid (graphite)
chlorine	Cl	greenish gas
chromium	Cr	silvery metal
cobalt	Co	silvery metal
copper (*cuprum*)	Cu	reddish metal
fluorine	F	pale yellow gas
gold (*aurum*)	Au	soft, yellow metal
helium	He	colourless gas
hydrogen	H	colourless gas
iodine	I	bluish-black solid
iron (*ferrum*)	Fe	silvery metal
lead (*plumbum*)	Pb	bluish metal
magnesium	Mg	silvery metal
manganese	Mn	grey metal
mercury (*hydrargyrum*)	Hg	silvery liquid
neon	Ne	colourless gas
nickel	Ni	silvery metal
nitrogen	N	colourless gas
oxygen	O	colourless gas
phosphorus	P	yellowish solid (white phosphorus)
potassium (*kalium*)	K	soft, silvery metal
silver (*argentum*)	Ag	silvery metal
sodium (*natrium*)	Na	soft, silvery metal
sulfur	S	yellow solid
zinc	Zn	bluish-white metal

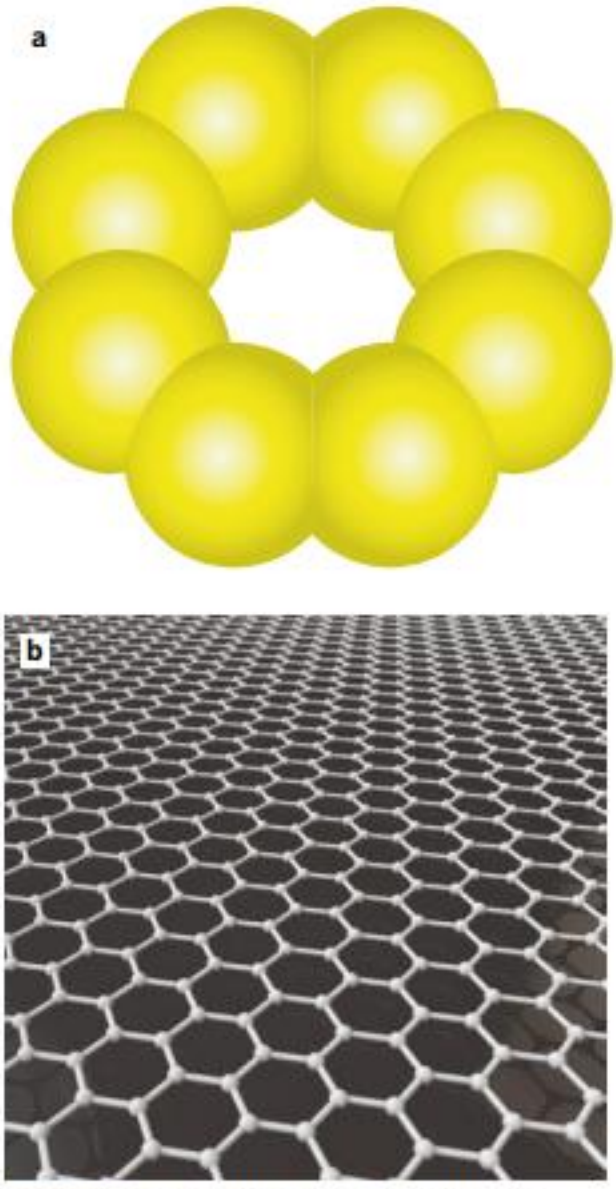


FIGURE 2.1.7 (a) Most non-metal elements, such as sulfur, form molecules. (b) Some elements, such as carbon, form covalent network lattices or giant covalent networks like the graphene shown here.

Along with a name and chemical symbol, each element is also assigned a number, called the **atomic number**. The atomic number identifies the number of protons in the atom. For our purposes, atomic numbers range from 1 (for hydrogen) up to 92 (for uranium), i.e. the 92 naturally occurring elements.

Other common physical properties used to describe pure substances are density, conductivity, tensile strength and expansion.

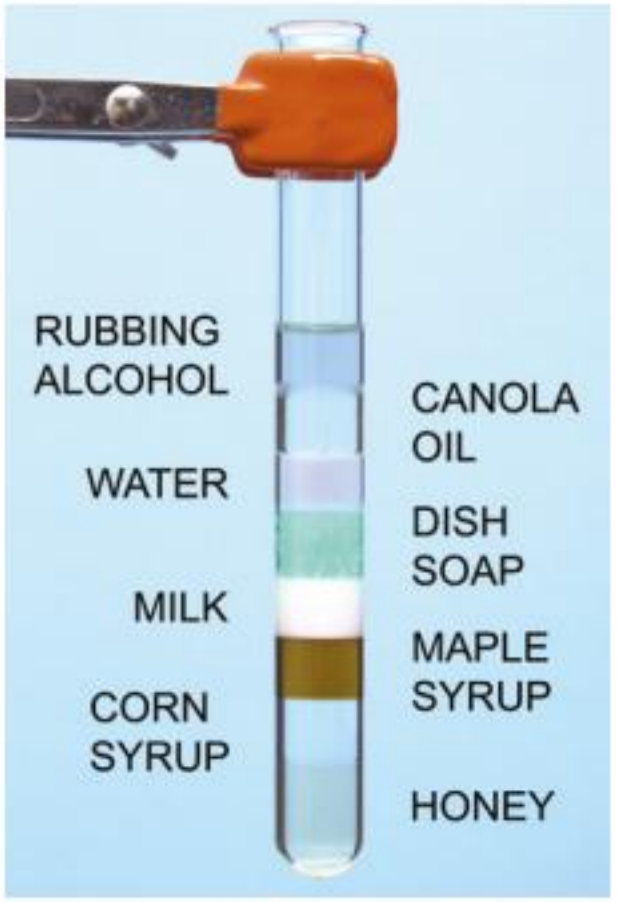


FIGURE 2.1.8 The relative density of some common liquids

i The periodic table is an arrangement of the elements in order of increasing atomic number in which elements of similar chemical and physical properties are placed in vertical columns known as groups.

Density is measured as the mass per unit volume. You will have observed substances with different densities in your everyday life. For example, a salad dressing made of oil and vinegar will have the oil floating on top of the vinegar because oil is less dense. Figure 2.1.8 shows the density of some common liquids. The liquids form layers in order of their density, with the least dense at the top and the most dense at the bottom.

Metals and metal alloys (mixtures) are used widely in manufacturing and construction. For many situations, such as in aeronautical engineering, manufacturers must consider the weight versus the strength that the metal provides. Table 2.1.3 shows the properties of some metals; for example, aluminium is a lightweight metal with relatively good strength.

TABLE 2.1.3 Some physical properties of common metal elements

	Density (g/cm³)	Thermal expansion (µm/m°C)	Electrical conductivity (MS/m)	Tensile strength (MPa)
gold	19.3	14.12	45.2	20
silver	10.5	18.9	63.0	170
copper	8.96	16.5	59.6	210
iron	7.87	11.8	10.4	300
aluminium	2.7	23.1	37.7	120
lead	11.3	29.1	4.81	17

The periodic table

Figure 2.1.9 shows that elements can be listed in a special way in the **periodic table of elements**. The periodic table groups elements with similar chemical and physical properties into vertical columns called **groups**. Most elements are metals, which appear on the left-hand side of the periodic table, while the non-metals appear towards the upper-right of the periodic table.

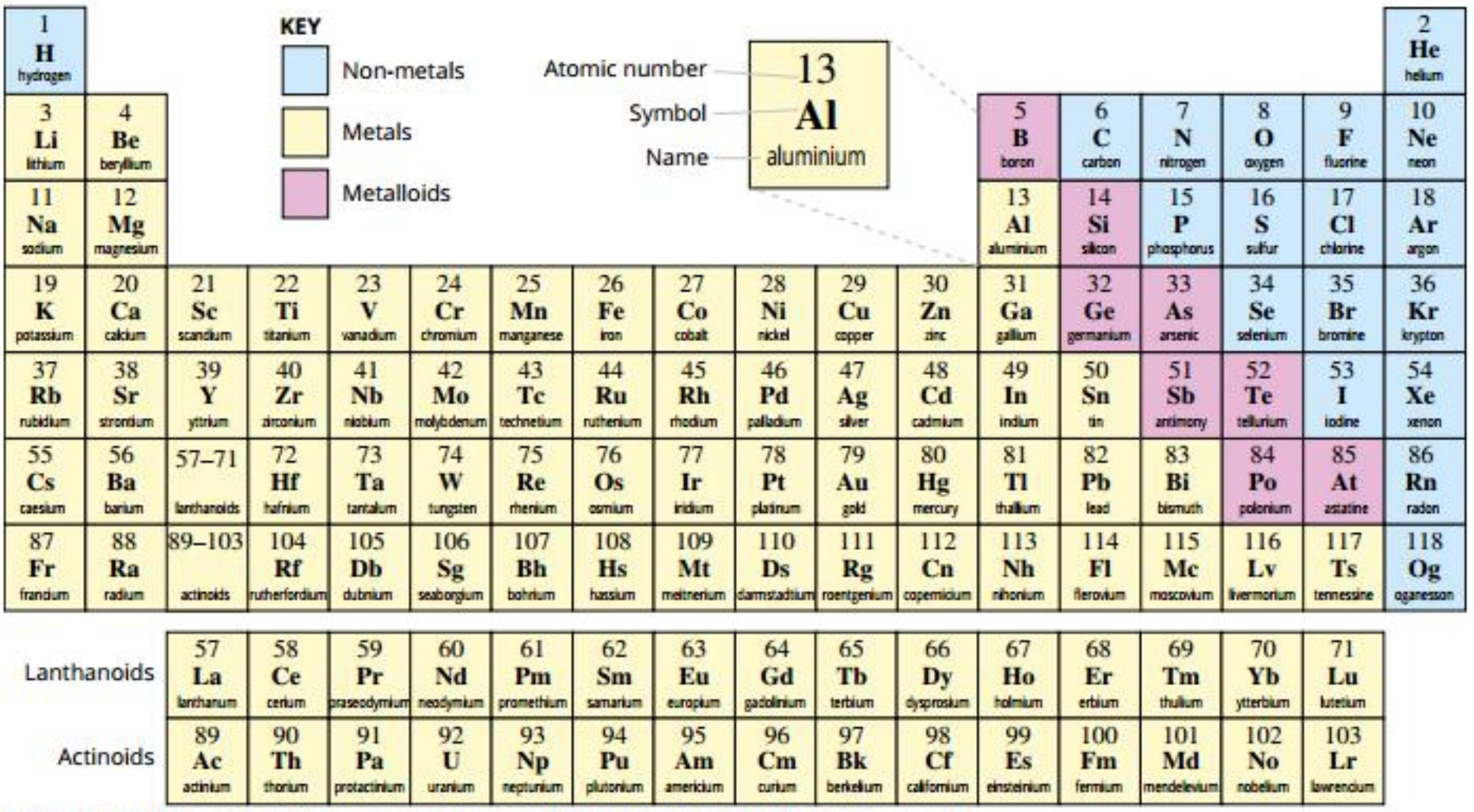


FIGURE 2.1.9 The periodic table groups elements according to their chemical and physical properties.

You will generally have a copy of the periodic table at hand during your chemistry studies so you don't need to memorise it in detail. However, being able to recall specific information about the first twenty elements or so is very useful. It is important to learn how to use the periodic table since it is the most useful tool in chemistry. There are many useful trends in the periodic table. For example, the atomic radius of each element in a period (row) decreases from left to right, and increases down each group (column). You will learn more about periodic table trends in Chapter 4.

COMPOUNDS

Compounds are substances formed from two or more elements in which the elements are always combined in the same fixed proportion. This means the composition of compounds does not vary, no matter how much of the compound there is. Water is a compound in which hydrogen and oxygen are always combined in the ratio of 2:1 and is represented by the chemical formula H_2O.

A **chemical formula** is a shorthand notation that uses elemental symbols from the periodic table, with numerical subscripts to convey the relative proportions of atoms of the different elements in the compound. You will note that the oxygen atom in the formula H_2O has no subscript. When an element in a chemical formula has no subscript, the subscript is presumed to be the number one.

Compounds are substances that can be broken down by chemical reactions to form other substances. To determine whether a pure substance is an element or a compound, you must determine if the substance can be broken down into elements. For example, when heated, mercury(II) oxide (HgO) decomposes to liquid mercury (Hg) and oxygen gas (O_2) (Figure 2.1.10). If it were not a compound, the mercury(II) oxide would not break down. As oxygen is a colourless gas, you cannot see it.

FIGURE 2.1.10 The red powder in this test tube is mercury(II) oxide (HgO). If you look closely at the test tube, you will see beads of liquid mercury forming from the decomposition of the compound.

Types of compounds

There are two major types of compounds: molecular compounds and ionic compounds. **Molecular compounds** are composed of molecules, all of which are alike and have non-metallic elements chemically bonded to other non-metallic elements in a fixed ratio. They tend to have relatively low boiling points and melting points. Examples of common molecular compounds include water (H_2O), methane (CH_4), ammonia (NH_3), benzene (C_6H_6), ethanol (C_2H_6O) and carbon dioxide (CO_2). Note how each example contains only non-metallic elements.

Ionic compounds form when metallic elements bond to non-metallic elements. Ionic compounds are composed of **ions** arranged in a rigid three-dimensional lattice. They contain positively charged ions (called **cations**) and negatively charged ions (called **anions**), which are attracted to each other by the electrostatic attraction of charges of opposite sign. They tend to have relatively high melting points and boiling points compared to molecular compounds. Examples of common ionic compounds include sodium chloride (table salt, NaCl), calcium carbonate (limestone, $CaCO_3$) and calcium oxide (lime, CaO). Note how each example contains a metallic cation and a non-metallic anion.

You will look at ionic compounds and molecular compounds in more detail in Chapters 7 and 8, respectively.

2.1 Review

SUMMARY

- Matter can be characterised and classified according to its purity.
- Pure substances are materials with definite and distinct chemical and physical properties.
- Mixtures are physical combinations of pure substances whose properties are dependent on the identity and relative amounts of the substances that make up the mixture.
- Changes in matter are brought about by physical or chemical changes: physical changes do not produce new substances; chemical changes result in the formation of new substances.
- Pure substances may be elements or compounds.
- Every element has a unique name, atomic number and chemical symbol.
- Elements are organised into the periodic table.
- Compounds are formed from two or more elements combined in the same fixed proportion.
- Molecular compounds are composed of non-metals bonded to other non-metals.
- Ionic compounds are composed of metals bonded to non-metals.

KEY QUESTIONS

Describe

1 Define the term 'matter'.

2 State two types of:
- **a** mixtures
- **b** pure substances.

3 Describe a physical change in matter.

4 Identify the common name of each of the following elements from its Latin name.
- **a** *ferrum*
- **b** *kalium*
- **c** *argentum*
- **d** *plumbum*
- **e** *hydrargyrum*

5 Select the correct terms to complete the following sentence.
Molecular compounds/ionic compounds are composed of non-metals bonded to non-metals, whereas *molecular compounds/ionic compounds* are composed of metals bonded to non-metals.

6 Name two physical properties that could be used to distinguish between these substances.
- **a** water and methanol
- **b** gold and copper
- **c** oxygen gas and chlorine gas

Apply

7 Pure water can be obtained from many different sources: rainwater, sea water and underground aquifers. Does the composition of pure water from different sources vary? Explain your answer.

8 Can both elements and compounds be molecules? Use appropriate examples to explain your answer.

9 Name the change of state associated with each of the following processes.
- **a** Water is made into ice cubes.
- **b** The inside of your car window fogs up.
- **c** Mothballs in the wardrobe disappear with time.
- **d** Wet washing dries.

10 Substance X is a silver-grey-coloured metal that melts at 420°C. When it is placed in dilute sulfuric acid, hydrogen is given off and the metal dissolves. It has a density of $7.13\,g\,cm^{-3}$ at 25°C and reacts slowly with oxygen to form a metal oxide. Describe the physical and chemical properties of substance X.

11 Explain the differences between an element, a compound and a mixture.

Analyse

12 Classify each of the following as a physical change or chemical change.
- **a** the evaporation of water
- **b** the rusting of iron
- **c** the grinding of salt crystals into powder
- **d** the burning of wood in a fireplace

13 Classify each of the following as an element, a compound or a mixture.
- **a** copper
- **b** sand
- **c** water
- **d** carbon dioxide
- **e** muddy water
- **f** sodium chloride
- **g** gold
- **h** lemonade

14 About 3.5% (3.5g per 100g) of the mass of sea water is the result of dissolved salts, mainly sodium chloride. Determine the freezing point of sea water using the graph in Figure 2.1.4b on page 7.

15 Classify each of the following elements on the periodic table on page 10 as a metal, metalloid or non-metal and represent each element using its chemical symbol.

- **a** magnesium
- **b** manganese
- **c** silver
- **d** mercury
- **e** neon
- **f** arsenic
- **g** sulfur
- **h** silicon

16 Classify the following as ionic compounds or molecular compounds using the periodic table on page 10.

- **a** NaCl
- **b** H_2S
- **c** PF_3
- **d** Fe_2O_3

17 Identify an element that has similar physical and chemical properties to potassium, K. Explain your reasoning.

18 Look at Table 2.1.3 (p. 10), which shows some physical properties of common metal elements, and use the information to answer the following questions.

- **a** Determine a metal that would be suitable for electrical wiring. Consider both electrical conductivity and cost in your answer.
- **b** Research the metals used in steel, a common construction metal alloy, and use the data in Table 2.1.3 to justify its composition.
- **c** Traditionally, sinkers used in fishing were made of lead. Environmentalists have argued against their use, because lost sinkers can be eaten by animals, which could poison them. Consider cost and other properties of lead, as well as the information in Table 2.1.3, to explain the popularity of lead sinkers.

19 A student is heating a clear liquid, presumed to be water, and finds it has a boiling point of 101.5°C. As the student continues to boil the liquid, the temperature rises to 103°C. Is the clear liquid pure water? Explain your answer.

2.2 Homogeneous and heterogeneous mixtures

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- discriminate between homogeneous and heterogeneous mixtures
- understand that the defining feature of a heterogeneous mixture is the presence of visually distinguishable phases that have different physical and chemical properties
- understand that liquid homogeneous mixtures, also known as solutions, are composed of solutes dissolved in a solvent.

Most samples of matter are not chemically pure and consist of a physical combination of two or more pure substances called a mixture. There are two types of mixtures—homogeneous mixtures and heterogeneous mixtures.

The terms **homogeneous** and **heterogeneous** have Greek origins: *homo*, meaning 'same', *hetero*, meaning 'different', and *genes*, meaning 'of a kind'. Homogeneous, therefore, translates to 'of the same kind' and heterogeneous translates to 'of a different kind'.

In some instances, mixtures are easily recognised. For example, consider a piece of granite, a choc-chip cookie and salad dressing (Figure 2.2.1). In these examples, you can see that different kinds of substances are present. In other cases, it is not so easy to recognise mixtures. For example, the air you breathe, sea water and sterling silver jewellery (Figure 2.2.2) may all appear to be pure but each consists of different substances. Air is a mixture of elements such as nitrogen (N_2) and oxygen (O_2) combined with compounds such as carbon dioxide (CO_2) and water vapour (H_2O); sea water is mostly a mixture of the compounds water (H_2O) and sodium chloride (NaCl); while sterling silver is a mixture of the elements silver (Ag) and copper (Cu). It is the uniformity of these mixtures and the lack of visibly different materials that make it hard for us to recognise them as mixtures.

FIGURE 2.2.1 Some examples of mixtures: (a) This sample of granite shows at least three visibly distinct regions—white quartz, orange feldspar and black mica minerals. (b) A choc-chip cookie has at least two visibly distinct regions. (c) Some salad dressings are made from oil and water.

FIGURE 2.2.2 Examples of matter that is not easily recognised as mixtures. (a) Air is a colourless mixture of nitrogen, oxygen and some trace gases. (b) Sea water is a colourless mixture of salt and water. (c) Sterling silver is a mixture of silver and copper but appears to be a single lustrous silver-coloured metal.

HETEROGENEOUS MIXTURES

The piece of granite, the choc-chip cookie and the salad dressing shown in Figure 2.2.1 are examples of heterogeneous mixtures. These samples of matter are not uniform throughout and you can clearly observe the presence of different types of materials. You also know from experience that the different parts of each of these mixtures have different properties, such as colour, taste and hardness.

Heterogeneous mixtures consist of two or more substances that have visibly distinguishable regions, called **phases**, which have different physical and chemical properties. A heterogeneous mixture is not uniform throughout, so two small samples obtained from different parts of the mixture would be different in composition.

Heterogeneous mixtures may have phases in the same physical state or in different physical states. Granite is a heterogeneous mixture of three solid phases—the white quartz mineral (i.e. silica, SiO_2), the orange feldspar mineral and the black mica mineral. The oil and water phases of salad dressing are also both in the same physical state—the liquid state. On the other hand, a sample of muddy water consists of solid dirt particles physically mixed with liquid water.

A phase is a region of matter that is physically and chemically uniform in composition and properties. It is physically distinct from other regions of matter and is mechanically separable from other phases.

HOMOGENEOUS MIXTURES

Homogeneous mixtures consist of a physical combination of two or more substances but have only one visibly distinct phase that has uniform properties. A homogeneous mixture is uniform throughout and samples taken from different parts of the mixture would be identical in composition. The air, sea water and sterling silver shown in Figure 2.2.2 are all examples of homogeneous mixtures where only one visibly distinct phase is observable.

Many homogeneous mixtures are also called **solutions** and have one substance dissolved in another. The substance present in the greatest amount is called the **solvent** and all other substances present in the mixture are called **solutes**. Solutes are said to be dissolved in the solvent.

The most common solutions you will encounter in your chemistry studies will be solid salts dissolved in liquid water (for example, sea water). The salts are the solutes and the water is the solvent. A solution in which water is the solvent is given the special name of an **aqueous solution**—the name being derived from the Latin *aqua*, meaning 'water'. Examples of some common solutions are shown in Table 2.2.1, which shows that solutions can involve mixtures across all three states of matter.

TABLE 2.2.1 Examples of common solutions

Example	States of matter involved	Solvent	Solute(s)	Physical appearance
air	gas–gas	nitrogen	oxygen, carbon dioxide, argon, water vapour	clear colourless gas
soft drinks	solid–liquid–gas	water	sugar, carbon dioxide gas	coloured liquid
vinegar	liquid–liquid	water	ethanoic acid	clear colourless liquid (white vinegar)
sea water	liquid–solid	water	sodium chloride plus other trace salts	clear colourless liquid
sterling silver	solid–solid	silver	copper	lustrous silver-coloured solid metal

Even though any single sample of a homogeneous mixture will be uniform throughout, the composition may vary from sample to sample, depending on the relative ratio of the substances in the solution. For example, two samples of salt water may be prepared by dissolving, firstly, one gram of salt in a litre of water and then, secondly, 10 grams of salt in a litre of water. Both salt water samples will be homogeneous throughout, but each sample will have different physical and chemical properties including density, electrical conductivity and boiling point.

2.2 Review

SUMMARY

- Most matter is not chemically pure and consists of a physical combination of two or more pure substances that form a mixture.
- Mixtures can be classified as heterogeneous or homogeneous mixtures.
- Heterogeneous mixtures have two or more visibly distinguishable regions, called phases, which have different physical and chemical properties. They are not uniform throughout.
- Homogeneous mixtures have only one visibly distinct phase. They are uniform throughout.
- Many homogeneous mixtures are known as solutions.
- Solutions consist of solutes dissolved in a solvent. When the solvent is water, the solution is known as an aqueous solution.
- Both heterogeneous and homogeneous mixtures can vary in composition from sample to sample and, therefore, can vary in chemical and physical properties.

KEY QUESTIONS

Describe

1 **a** Define the term 'phase' with respect to heterogeneous and homogeneous mixtures.
b State how many phases all solutions have.

2 Define the terms 'solution', 'solvent' and 'solute'.

3 Determine if the following statements about mixtures are true or false.
a Mixtures can be separated based on their physical properties.
b It is possible to see the individual components in a salt solution.
c Heterogeneous mixtures always have phases in the same physical state.
d In an aqueous solution, the solvent is water.

Apply

4 Explain the difference between a heterogeneous mixture and a homogeneous mixture, using suitable examples.

5 Describe the key components of a copper sulfate solution (shown below), and explain why it is uniform.

Analyse

6 Classify each of the following as a homogeneous or heterogeneous mixture.
a muesli
b sand
c wet sand
d vinegar

7 Differentiate between a *state* of matter and a *phase* of matter.

8 Identify which of the following can have a varied composition. Explain your answer in each case.
a element
b compound
c homogeneous mixture
d heterogeneous mixture

9 Identify the following metallic substances as elements or mixtures.
a brass
b sterling silver
c bronze
d mercury
e gold
f iron

10 For each of the following solutions, identify the component as a solvent or solute.

Component in solution	Solvent or solute?
a oxygen in air	
b water in sea water	
c copper in sterling silver	

11 In the laboratory, a student compares the properties of two unknown mixtures. The results of the experiment are shown in the table below.

	Mixture A	Mixture B
Appearance	clear blue liquid	speckled grey/ black solids
States of matter present	liquid only	solid only
Number of phases	one	two

Classify mixtures A and B as homogeneous or heterogeneous. Give evidence to support your answer.

Chapter review

02

KEY TERMS

alloy
anion
aqueous solution
atom
atomic number
boiling point
boiling point elevation
cation
chemical change
chemical equation
chemical formula
chemical reaction
chemical symbol
compound
covalent network lattice
density
element
freezing point
freezing point depression
giant covalent network
group
heterogeneous
heterogeneous mixture
homogeneous
homogeneous mixture
ion
ionic compound
mass
matter
mixture
molecular compound
molecule
periodic table of elements
phase
physical change
physical property
physical state
pure substance
solute
solution
solvent
volume

KEY QUESTIONS

Describe

1 Select the response that best describes a sample of matter that has these three characteristics.
- It is uniform throughout.
- It cannot be separated into other substances by physical processes.
- It can be decomposed into other substances by chemical processes.

A a heterogeneous mixture
B a homogeneous mixture
C an element
D a compound

2 Identify the following as either a chemical property or a physical property of matter.
a boiling point
b melting point
c combustibility
d toxicity
e density

3 Name the vertical columns of the periodic table. State their significance.

4 Select the list below that contains only pure substances.
A tap water, air, ammonia
B air, hydrogen gas, glucose
C distilled water, glucose, sand
D ammonia, glucose, distilled water

5 Select the list below that contains only homogeneous mixtures.
A air, amalgam, seawater
B air, tap water, pizza
C copper, gold, oxygen
D choc-chip cookies, concrete, wine

6 Which of the following is an indicator of a chemical change?
A A solid dissolves in water.
B A precipitate is formed.
C There is a change in state.
D There is a change in viscosity when heated.

Apply

7 Which of the following can have a varied composition throughout a sample?
A element
B compound
C homogeneous mixture
D heterogeneous mixture

8 Below are four samples of different matter. Which of the samples are heterogeneous mixtures?
I iron ore
II copper wire
III wet sand
IV distilled water
A I and II
B II and III
C III
D I and III

9 Determine which of the following are pure substances and which are mixtures. For each, list all of the different phases present.
a paint, containing a liquid solution and a dispersed solid pigment
b partially molten copper

10 Describe the key difference between a physical change and a chemical change.

11 There is a range of liquid metal alloys containing gallium, indium, tin, zinc and silver. In their elemental state, all of these metals are solid. Explain why the alloy has different properties to the individual elements.

12 Natural gas used in the home for heating and cooling is composed mainly of methane CH_4 and ethane C_2H_6. It can have small traces of other gaseous substances present. Both methane and ethane are odourless and colourless gases, but when a gas tap is left on, there is a distinct odour present. This is due to the addition of warning agents, which have distinct odours. Ethanethiol (CH_3CH_2SH), a liquid at room temperature, is one such warning agent.

- **a** Are methane and ethane elements or compounds? Explain your answer.
- **b** State three physical properties of ethane.
- **c** State one chemical property of methane.
- **d** Is natural gas a homogeneous or heterogeneous mixture?
- **e** State two physical properties of ethanethiol.

13 Draw particle diagrams to explain the difference between a diatomic element and a monatomic element.

Analyse

14 Classify each of the following pure substances as elements or compounds, based on the information given, or indicate that no such classification is possible because of insufficient information.

- **a** Analysis indicates that substance A contains two elements.
- **b** Substance B decomposes upon heating.
- **c** Heating substance C to 900°C causes no change.
- **d** Heating substance D to 400°C causes it to melt.

15 The following is a description of the element cadmium (Cd).

I It is a bluish-white coloured lustrous metal.
II It has a melting point of 321°C.
III When added to hydrochloric acid, the metal dissolves and hydrogen gas is released.
IV It is highly toxic and can adversely affect the kidneys, lungs and bones.
V It has a density of $8.65\,g\,cm^{-3}$.
VI It has a hardness of 2.0 on the Moh hardness scale.
VII If left in air, it will form a layer of cadmium oxide (CdO) on its surface.

Which of the following are chemical properties of cadmium?

A I, III and IV
B III, IV and VII
C III, IV and VI
D IV, VI and VII

16 Classify each of the following changes as a physical change or a chemical change.

- **a** the evaporation of ethanol
- **b** the rusting of steel
- **c** the grinding of sugar crystals into powder
- **d** the burning of coal in a fireplace

17 Below is a list of changes.

I corrosion of zinc anodes on boats
II melting of iron in a blast furnace
III pulverising of a granite sample
IV digesting chocolate
V growth of plants via photosynthesis
VI explosion of TNT

Which of the following are physical changes?

A I, II and III
B II, III and IV
C II and III
D III and V

18 Compare and contrast elements and compounds.

19 Identify the elements in the following molecular compounds, writing their name, symbol and atomic number.

- **a** ammonia (NH_3)
- **b** benzene (C_6H_6)
- **c** dinitrogen pentoxide (N_2O_5)

20 Identify what you note about the nature of the elements in the compounds listed in Question **19** and what type of compound they are.

21 Identify the elements in the following ionic compounds, writing their name, symbol and atomic number.

- **a** calcium fluoride (CaF_2)
- **b** aluminium oxide (Al_2O_3)
- **c** copper(I) sulfate (Cu_2SO_4)

22 Identify what you note about the nature of the elements in the compounds listed in Question **21** and what type of compounds they are.

23 If you light a match under a cold metal spoon you may observe one or more of the following. Classify each observation as a physical change or a chemical change.

- **a** The match burns.
- **b** Carbon soot is produced.
- **c** The metal spoon gets warmer.
- **d** Water condenses on the metal spoon.
- **e** Carbon soot is deposited on the metal spoon.

24 Determine all possible answers for each scenario from the list below.

- compound
- element
- heterogeneous mixture
- homogeneous mixture

a matter that cannot be broken down into simpler substances by chemical or physical means

b matter that can be separated into its constituent components by physical processes

c matter that can only be separated into its constituent components by chemical processes

25 Identify the solvent and solute(s) in the following solutions.

a air

b sea water

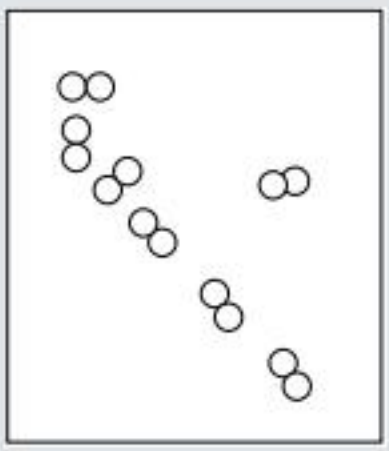
c vinegar

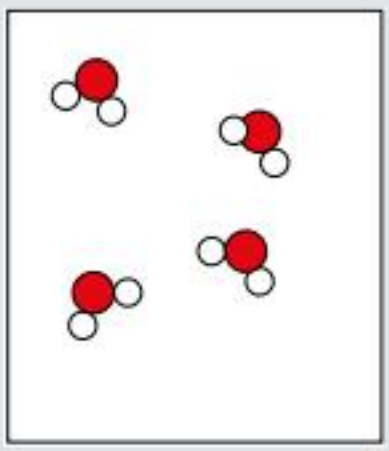
d white wine

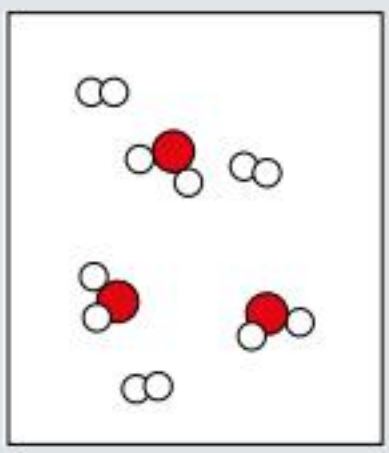
e fish tank water

26 A student is investigating an unknown grey solid and begins by testing its melting point. They find the solid has a melting point range of 189–193°C. What conclusions can be drawn about the purity of the solid?

27 The diagram below shows molecules of two different elements. Classify A, B and C as element, compound or mixture.







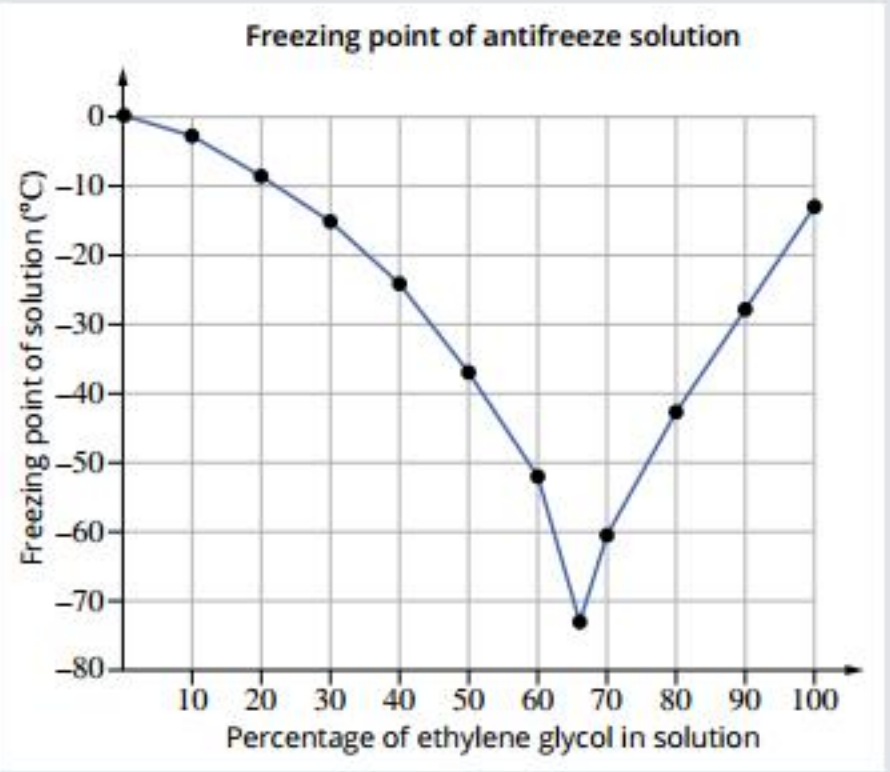
Interpret

28 A glass contains a clear, colourless liquid that looks like water. Develop a test to describe how you can be sure that, if it is water, it is pure and does not contain any dissolved salts.

29 Ethylene glycol is used as an antifreeze additive in vehicle radiators to stop the radiator water from freezing in cold weather. The lowest ever recorded temperature in Australia is −23.4°C recorded at Charlotte's Pass in the NSW Snowy Mountains on 29 June 1994. Use the following graph to answer these questions.

a Decide what percentage concentration of ethylene glycol would be required to be confident that a vehicle radiator would not freeze in Australia.

b The lowest recorded temperature in Canberra is −10°C. Determine what percentage concentration of ethylene glycol would be required to be confident that a vehicle radiator would not freeze in Canberra.



30 Two students are investigating mixtures. They have access to water, table salt (sodium chloride), sand, glass beads and sugar. They are told that each mixture must contain a minimum of three of the substances.

a Student 1 is tasked with making a heterogeneous mixture. They add a small quantity of table salt, sand and several glass beads to a beaker and label it mixture 1. Have they succeeded in their task? Explain your answer.

b Student 2 is tasked with making a homogeneous mixture. They add some water to mixture 1, and claim it is a solution. Have they succeeded in their task? Explain your answer.

c Propose a method to satisfy the task of making a homogeneous mixture with three of the substances.

Data analysis

DATA SET 1

The information below applies to Questions 1–5.

Solder is an alloy most often made from tin and lead in different ratios. One of its common uses is to hold components in place in electric circuits. The advantage of solder is that it has a lower melting point than either of its component metals. This means that it will melt easily when it comes into contact with a soldering iron, then solidify quickly to hold components in place.

FIGURE 1 A soldering iron used to melt solder

A student investigated the change in the melting point as the percentage of tin is increased in the tin/lead alloy. Table 1 shows the data the student collected for the melting point of alloys made with varying percentages of tin.

TABLE 1 Melting point of alloys

Percentage of tin by mass	Melting point (°C)
10	302
20	280
30	258
40	238
50	214
60	190
70	192
80	202
90	216

Question 1 (2 marks)

Name the independent variable and the dependent variable for this investigation.

Question 2 (4 marks)

Plot the data in Table 1 in an appropriate graph.

Question 3 (2 marks)

Describe the trend shown by the data.

Question 4 (1 mark)

Identify the percentage of tin that provides the lowest melting point.

Question 5 (2 marks)

Examining the data, does it verify that mixtures have varying properties dependent on the identity and relative amounts of the substances that make up the mixture? Explain your answer.

CHAPTER

03 The atomic world

In this chapter, you will develop a detailed knowledge of the internal structure of atoms, which are the fundamental building blocks of matter and the foundation for all chemistry.

You will learn that some elements are composed of different types of atoms, called isotopes. Some isotopes are both useful and potentially harmful because they are unstable and release radiation when they decay.

Many of the details of atomic structure that are described in this chapter were discovered just 100 years ago when physicists and chemists made numerous ground-breaking experimental and theoretical observations—each one contributing to our understanding of the invisible world inside atoms.

Syllabus subject matter

Topic 1 • Properties and structure of atoms

■ ATOMIC STRUCTURE

- Describe that atoms can be modelled as a nucleus surrounded by electrons in distinct energy levels. **3.1**
- Discriminate between the terms *atomic number* (Z), *mass number* (A) and *isotopes of an element*. **3.2**
- Apply the nuclear symbol notation ${}^{A}_{Z}\mathrm{M}$ to determine the number of protons, neutrons and electrons in atoms, ions and isotopes. **3.2**
- State the relative energies of the s, p and d orbitals. **3.3**
- Apply the Aufbau principle, Hund's rule and the Pauli exclusion principle to write electron configurations for atoms and ions up to $Z = 36$. **3.3**
- Determine full and condensed electron configurations for atoms and ions up to $Z = 36$, e.g. $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^5$ and $[Ne]3s^2\ 3p^5$. **3.3**
- Identify the electron configuration of Cr and Cu as exceptions. **3.3**
- Explain how successive ionisation energy data is related to the electron configuration of an atom. **3.1**

■ ISOTOPES

- Describe that isotopes are atoms of the same element that have different numbers of neutrons. **3.2**
- State that isotopes can be represented in the form ${}^{A}\mathrm{X}$ (IUPAC) or X-*A*. **3.2**
- Identify that isotopes of an element have the same electron configuration and possess similar chemical properties but have different physical properties. **3.2**
- Explain that the relative atomic mass of an element is the ratio of the weighted average mass per atom of the naturally occurring form of the element to $\frac{1}{12}$ the mass of an atom of carbon-12. **3.2**

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3.1 Inside the atom

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand how the current model of the atom shows that it is composed of three types of subatomic particles (protons, neutrons and electrons) held together by electrostatic attraction
- describe each subatomic particle's mass, charge and position in the atom
- recall that elements are defined by the number of protons—the atomic number. The mass number is the number of particles in the nucleus (protons and neutrons)
- understand that most of the mass is in the nucleus and that the cloud of electrons is arranged in shells, each one having a particular energy level
- understand that the lower energy shells are closer to the nucleus and that energy is given off or absorbed when an electron moves to a different shell of lower or higher energy
- recall the defined number of electrons that can exist in each shell
- relate the size of ionisation energy to the shell of an electron.

Over time, scientists have gained a deep understanding of the structure of **atoms**, which are the basic building blocks of **matter**. As scientists' understanding has increased, their ability to control matter on the atomic scale has also improved. However, atoms are too small to be seen and so much of what scientists know about atoms has come from theoretical models and indirect experimental observations. More detail on historical experiments is provided in Module 3.3.

STRUCTURE OF ATOMS

All atoms are made up of a small, positively charged nucleus surrounded by a much larger cloud of negatively charged **electrons**, as shown in Figure 3.1.1. The **nucleus** is in turn made up of two types of **subatomic particles—protons** and **neutrons**. The protons are positively charged and the neutrons have no charge.

A scientific model is a description that scientists use to represent the important features of what they are trying to describe. This is based on experimental observations. They can then test the consistency of their observations against various predictions of the model.

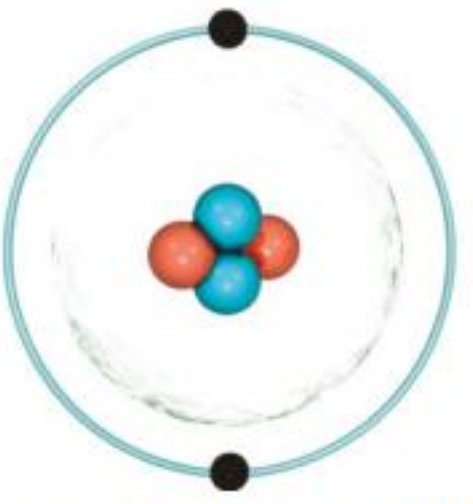


FIGURE 3.1.1 A simplified model of the atom. This shows a helium atom with two protons and two neutrons (in the central nucleus) and two electrons (in the outer ring). The outer ring symbolises that the electrons are held in an orbit; however, evidence suggests that they move throughout a region of space that is more like a cloud.

The nucleus

The nucleus of an atom is approximately 10000–100000 times smaller than the size of the atom. To put this in perspective, if an atom were the size of the Woolloongabba Cricket Ground (Figure 3.1.2), then the nucleus would be about the size of a pea. Nonetheless, the nucleus contributes around 99.97% of the atom's mass. This means that atomic nuclei are extremely dense.

FIGURE 3.1.2 If an atom were the size of the Woolloongabba Cricket Ground, then the nucleus would be the size of a pea, and the electrons would be found in a stadium-sized cloud.

The subatomic particles in the nucleus, protons and neutrons, are referred to collectively as **nucleons**. Protons are positively charged particles with a mass of approximately 1.673×10^{-27} kg or 1 atomic mass unit (amu). Neutrons and protons are almost identical in mass. Table 3.1.1 summarises the properties of protons, neutrons and electrons.

TABLE 3.1.1 Properties of the subatomic particles

Particle	Symbol	Charge	Mass relative to a proton	Mass (kg)
proton	p	+1	1	1.673×10^{-27}
neutron	n	0	1	1.675×10^{-27}
electron	e	−1	$\frac{1}{1800}$	9.109×10^{-31}

Electrons

Electrons are negatively charged particles. You can imagine them forming a cloud of negative charge around the nucleus. This cloud gives the atom its size and volume.

An electron is approximately 1800 times lighter than a proton or neutron. Therefore, electrons contribute very little to the total mass of an atom. However, the space occupied by the cloud of electrons is 10000–100000 times larger than the nucleus.

Positive particles attract negative particles. This is called **electrostatic attraction**. Electrons are bound to the nucleus by electrostatic attraction to the protons within the nucleus. The charge of an electron is equal to but opposite the charge of a proton. Electrons are said to have a charge of −1, whereas protons have a charge of +1. This means that all neutral **elements** have equal numbers of protons and electrons, and therefore have no electrical charge.

In some circumstances, electrons can be removed from an atom. For example, when you rub a rubber balloon on a woollen jumper or dry hair, electrons are transferred to the balloon and the balloon develops a negative charge. The negative charge is observed as an electrostatic force that can stick the balloon to a wall or even move an aluminium can. You will look more closely at the removal of electrons from atoms when learning about ionic compounds in Chapter 7.

The electricity that powers lights and appliances is the result of electrons moving in a current through wires. Sparks and lightning are also caused by electrons moving through the air.

ELECTRON SHELLS

Beginning with the hydrogen atom and extending to many other elements, scientists in the early 20th century observed energy being released in 'packets' or **quanta** (observed as particular wavelengths of light). Niels Bohr proposed that electrons were grouped into different **energy levels**, called **electron shells**.

In the **shell model** (which is also called the **Bohr model**), the shell in which an electron is located depends on the energy of the electron; electrons with low energy are located in shells close to the nucleus, while high-energy electrons are located in outer shells (Figure 3.1.3). Due to the difference in energy levels between shells, if an electron moves to a different shell, energy must be absorbed or released. Electrons in the same shell share the following characteristics:

- They are about the same distance from the nucleus.
- They have about the same energy.

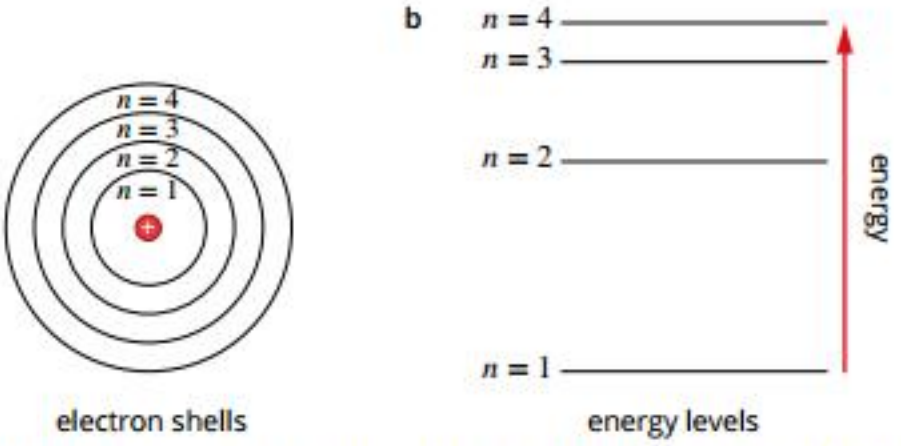


FIGURE 3.1.3 (a) In the Bohr model, the electron shells are labelled using integers (n). The first shell is the shell closest to the nucleus and the radii of the shells increase as the shell numbers increase. (b) Each shell corresponds to an energy level that electrons can occupy. The first shell has the lowest energy level and the energy level increases as the shell number increases.

The lowest energy shell is the shell closest to the nucleus and is labelled $n = 1$. Shells with higher values of n correspond to higher energy levels (Figure 3.1.3). As the values of n increase, the energy levels get closer together.

When fireworks explode, they create a spectacular show of coloured lights (Figure 3.1.4). The light is produced by metal atoms that have been heated by the explosion. When they are heated, electrons 'jump' to a higher energy level (**excited state**) and then release light energy as they return to their lower energy level (**ground state**). This process creates different colours (wavelengths) of light because each metal element has a different electron arrangement. These unique **emission spectra** are further described in Chapter 5.

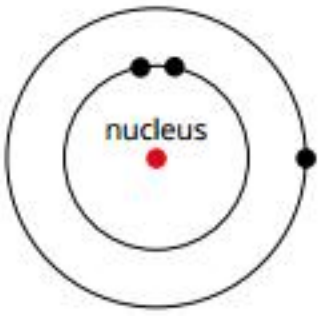
FIGURE 3.1.4 The spectacular colours from a New Year's Eve fireworks display in Brisbane. As metal atoms are heated to very high temperatures during the explosion that launches the firework, some of their electrons are moved to higher energy levels. As the electrons return to lower energy levels in the metal atoms, light of a particular wavelength (colour) is emitted.

In all atoms, the electrons are as close to the nucleus as possible. This means that electrons will generally occupy inner shells before outer shells. For example, an atom of lithium has three electrons. Two electrons will occupy the $n = 1$ shell as that is all it can hold. The third electron is in the $n = 2$ shell.

A **Bohr diagram** is a simple diagram that shows the arrangement of electrons around the nucleus. In such diagrams, only the shells that are occupied are drawn. A Bohr diagram for lithium is shown in Figure 3.1.5.

You have learnt that each shell has a particular energy level. These shells will only hold a particular number of electrons. The maximum number of electrons that a shell can hold can be calculated using $2n^2$, where n is the shell number. For example, for the $n = 1$ shell, $2n^2$ is two electrons; whereas for the $n = 2$ shell, $2n^2 = 8$ electrons.

It is possible to determine the arrangement of electrons in the shells of any atom since each shell can only contain a maximum number of electrons. Table 3.1.2 shows how many electrons can occupy the first four shells.



Li 2,1

FIGURE 3.1.5 A Bohr diagram showing the electron shells of the lithium atom (containing three electrons). Protons and neutrons are not shown.

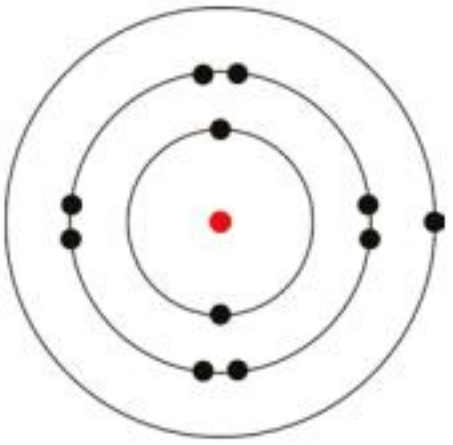
TABLE 3.1.2 The number of electrons held by each shell of an atom. Shell $n = 1$ is the shell closest to the nucleus.

Electron shell (n)	Maximum number of electrons
1	2
2	8
3	18
4	32
n	$2n^2$

An oxygen atom has eight electrons, so its $n = 1$ shell will hold two electrons and its $n = 2$ shell will hold six electrons.

From the third shell onwards, even though the shells can hold more than eight electrons, the outermost shell has a maximum of eight electrons. For example, the electron arrangement for potassium ($Z = 19$) is 2,8,8,1, not 2,8,9. Once the third shell reaches eight electrons, the next shell starts filling.

Figure 3.1.6 shows a Bohr diagram of a sodium atom, which has 11 electrons. The first two electrons fill the $n = 1$ shell. The next eight electrons fill the $n = 2$ shell. The remaining electron occupies the $n = 3$ shell. The arrangement of the electrons in the shells can be written as 2,8,1.



Na 2,8,1

FIGURE 3.1.6 A Bohr diagram of the arrangement of electrons in the shells of a sodium atom

Worked example 3.1.1

ARRANGEMENTS OF ELECTRONS IN SHELLS (FOR UP TO 18 ELECTRONS)

Apply the rules of the shell model to determine the arrangement of electrons in the shells of an atom with 16 electrons.

Thinking	Working
Recall the maximum number of electrons that each shell can hold. Remember that the outermost shell can hold no more than eight electrons.	shell (n) — maximum number of electrons 1 — 2 2 — 8 3 — 18
Place the 16 electrons in the shells from the lowest energy to the highest energy. Do not exceed the maximum number of electrons allowed in each shell. Note that $n = 3$ could hold 18 electrons, but in this atom, it only has 6 electrons.	shell (n) — electrons in shell 1 — 2 2 — 8 3 — 6
Write the arrangement of electrons in the shells.	The arrangement of electrons in the shells can be written as 2,8,6.

➤ Try yourself 3.1.1

ARRANGEMENTS OF ELECTRONS IN SHELLS (FOR UP TO 18 ELECTRONS)

Apply the rules of the shell model to determine the arrangement of electrons in the shells of an atom with 13 electrons.

Valence electrons

The outermost shell of an atom is known as the atom's **valence shell**. The electrons in the outermost shell are called **valence electrons**. The valence electrons are involved in chemical reactions. Consequently, if you know the number of valence electrons in the atoms of an element, then you can predict the chemical properties of the element and the bonds that it will form.

In Chapters 7 and 8, you will learn how atoms tend to lose, gain or share valence electrons to achieve eight electrons in their valence shell when they bond with other atoms. This is known as the **octet rule**. The arrangement of elements in the **periodic table** is closely linked to the number of valence electrons in the atoms of each element (see Chapter 4).

Worked example 3.1.2

CALCULATING THE NUMBER OF VALENCE ELECTRONS IN AN ATOM

Determine the number of valence electrons present in an atom of magnesium, which has an atomic number of 12.

Thinking	Working
Recall the maximum number of electrons that each shell can hold. Remember that the outermost shell can hold no more than eight electrons.	shell (n) — maximum number of electrons 1 — 2 2 — 8 3 — 18
Place the 12 electrons in the shells from the lowest energy to the highest energy. Do not exceed the maximum number of electrons allowed in each shell.	shell (n) — electrons in shell 1 — 2 2 — 8 3 — 2
Determine the number of valence electrons by identifying the number of electrons in the valence shell (outermost shell).	The number of electrons in the valence shell is two. Therefore, magnesium has two valence electrons.

➤ Try yourself 3.1.2

CALCULATING THE NUMBER OF VALENCE ELECTRONS IN AN ATOM

Determine the number of valence electrons present in an atom of phosphorus, which has an atomic number of 15.

IONISATION ENERGY

The **ionisation energy** is the energy needed to remove an electron from an atom. Removing electrons that are located in the outermost shell requires less energy than removing electrons located in shells that are closer to the nucleus. For example, a sodium atom contains 11 electrons and the arrangement of electrons in its shells is 2,8,1. As each successive electron is removed (one by one), these ionisation energies can be measured. Figure 3.1.7 shows that the first electron to be removed has the lowest ionisation energy. The first electron is easiest to remove because it is in the outermost shell, $n = 3$. The following eight electrons are in the $n = 2$ shell and are more difficult to remove. Finally, the last two electrons require substantially more energy to remove as they are in the innermost shell, $n = 1$. In this position, closer to the nucleus, the electrostatic attraction is much greater, which means that much more energy needs to be used to remove each electron.

Removing electrons from atoms provided evidence for the existence of energy levels in atoms. Once scientists had determined the successive ionisation energies for many elements, they concluded that electrons were grouped into different energy levels. Figure 3.1.7 shows three energy levels in the sodium atom. The evidence for this is that the second to ninth electrons (in the $n = 2$ shell) need a similar amount of energy to be removed (ionised); there is a large increase in energy required after the first electron has been removed (in the outermost shell, $n = 3$), and again to remove the last two electrons (after the ninth electron) from the innermost shell, $n = 1$. This pattern in the ionisation energies is evidence of the different energy levels of each shell.

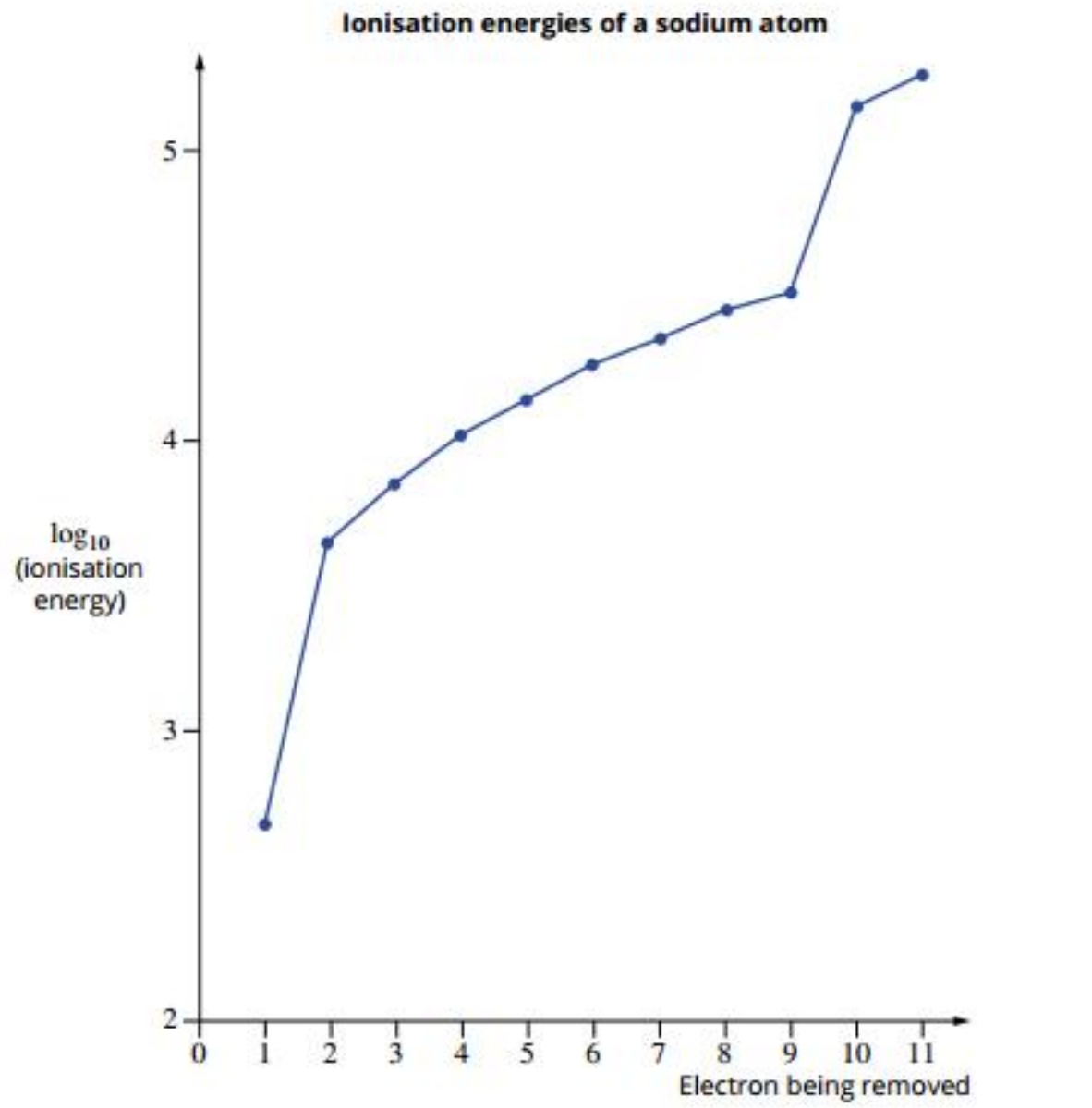


FIGURE 3.1.7 This graph of the ionisation energies of a sodium atom provides evidence for the arrangement of electrons in shells within atoms. (The logarithm of ionisation energy is used to provide a more convenient vertical scale.)

3.1 Review

SUMMARY

- All atoms are composed of a small, positively charged nucleus surrounded by a negatively charged cloud of electrons.
- The mass of an atom is mostly determined by the mass of the nucleus, while the size of an atom is determined by the cloud of electrons.
- The nucleus is made up of two subatomic particles called nucleons—protons and neutrons.
- Protons have a positive charge, electrons have a negative charge and neutrons have no charge.
- Protons and neutrons are similar in size and mass, while electrons are approximately 1800 times smaller.
- The shell model (Bohr model) of an atom assumes that electrons can only exist in fixed, circular orbits of specific energies called energy levels or shells.
- Lower energy shells are closer to the nucleus and other shells are like layers of an onion around the nucleus.
- The maximum number of electrons that can exist in a shell (n) is given by $2n^2$. This means that the $n = 1$ shell, $n = 2$ shell and $n = 3$ shell could hold 2, 8 and 18 electrons, respectively.
- The arrangement of electrons in shells in an atom can be written as a series of numbers separated by commas, e.g. 2,8,2.
- When an electron absorbs energy (e.g. heat or light), the electron can jump from a lower energy shell to a higher energy shell.
- When an electron falls from a higher energy shell to a lower energy shell, it can emit energy in the form of light.
- The outermost electron shell is called the valence shell and electrons in the outermost shell are called valence electrons. The valence shell cannot contain more than eight electrons.
- The ionisation energy (energy required to remove an electron) is greater for electrons in shells closer to the nucleus.

KEY QUESTIONS

Describe

1 How many times larger is an atom than its nucleus?

2 Describe how electrons are held within the cloud surrounding a nucleus.

3 Describe what energy change occurs when an electron in an atom moves from a higher energy shell to a lower energy shell.

4 Explain the meaning of the term 'ionisation energy'.

Apply

5 State the number of electrons in each shell for atoms with the following number of electrons.

a 5 electrons

b 12 electrons

c 17 electrons

6 How many valence electrons are there in an atom that has 18 electrons?

7 Draw Bohr diagrams for atoms of carbon and argon.

8 Determine the electron arrangement in the shells of atoms of the following elements.

a Be

b S

c Mg

9 A lithium atom has two electrons in the first shell and one electron in the second shell. Which shell would be the first to lose an electron when this atom is ionised? Explain your answer.

Analyse

10 Use Table 3.1.2 on page 25 to calculate the maximum number of electrons that can reside in the fifth and sixth shells of an atom.

11 **a** Consider the ionisation energy data for aluminium shown below and represent this on a graph similar to the graph shown in Figure 3.1.7 on page 28.

b Explain how this data reflects the arrangement of electrons in the shells of an aluminium atom.

Ionisation number	Ionisation energy ($kJ\,mol^{-1}$)
1	577.5
2	1816.7
3	2744.8
4	11577.0

3.2 Nuclear symbol notation

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- write the nuclear symbol notation for elements using atomic number and mass number
- determine the number of subatomic particles in an atom from an element's atomic number and mass number
- recall that isotopes are atoms of the same element that have different numbers of neutrons and can be represented in the form ^{A}X (IUPAC notation) or X-*A*
- recognise that isotopes of an element have the same electron shell arrangements and possess similar chemical properties, but have different physical properties
- understand the origin of radioactivity and the usefulness of radioisotopes, and some potential risks associated with their use.

An element is made up of one type of atom. The type of atom that makes up each element is determined by the number of protons in the nucleus. So, for example, an atom of carbon will always have six protons. In the unlikely event that a carbon atom loses a proton, it is no longer a carbon atom—it has become a boron atom. However, this is not true for electrons and neutrons—sometimes these particles are lost or gained. If a carbon atom, for example, loses or gains a neutron, the atom becomes an alternative form of carbon, called an **isotope**. To simplify the description of how many of each type of subatomic particle—protons, neutrons and electrons—are present in an atom, scientists use nuclear symbol notation.

ATOMIC NUMBER AND MASS NUMBER

The number of protons in an atom's nucleus is known as its **atomic number** and is represented by the symbol Z. All atoms of the same element have the same number of protons and therefore have the same atomic number. For example, all hydrogen atoms have $Z = 1$, all carbon atoms have $Z = 6$ and all gold atoms have $Z = 79$.

The number of protons and neutrons (nucleons) in the nucleus is known as the **mass number** and is represented by the symbol A. The mass number is obtained by adding the number of protons to the number of neutrons and represents the total mass of the nucleus.

Atoms are electrically neutral because the number of protons in an atom is equal to the number of electrons in the atom, which balances out the total positive and negative charges. The atomic number therefore tells you both the number of protons and the number of electrons in a neutral atom. For example, carbon atoms, with $Z = 6$, have six protons and six electrons.

In a neutral atom, number of protons = number of electrons.

Similarly, by definition, if the atomic number and mass number are known for a particular atom, the number of neutrons can be calculated. The number of neutrons is equal to the mass number (which is the total number of protons and neutrons) minus the atomic number (number of protons).

Number of neutrons = mass number – atomic number

The number of protons, neutrons and electrons defines the basic structure of an atom. **Nuclear symbol notation** represents an atom using its atomic number and mass number, as shown in Figure 3.2.1. This notation includes the mass number as a superscript and the atomic number as a subscript.

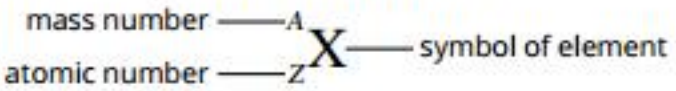


FIGURE 3.2.1 Nuclear symbol notation showing the atomic number and mass number of an atom

For an aluminium atom, the nuclear symbol notation would be written as shown in Figure 3.2.2.

$^{27}_{13}Al$

FIGURE 3.2.2 This representation of an aluminium atom indicates the number of protons, neutrons and electrons in the atom.

From this notation, you can determine that:

- aluminium has 13 protons ($Z = 13$)
- aluminium has 14 neutrons (mass number minus atomic number, $A - Z = 27 - 13$)
- aluminium has 13 electrons because uncharged atoms have no overall charge, so the number of electrons equals the number of protons.

Worked example 3.2.1

CALCULATING THE NUMBER OF SUBATOMIC PARTICLES

Calculate the number of protons, neutrons and electrons for the atom with this nuclear symbol:

$^{40}_{18}Ar$

Thinking	Working
The atomic number is equal to the number of protons.	the number of protons = $Z = 18$
Find the number of neutrons. Number of neutrons = mass number − atomic number	the number of neutrons = $A - Z$ $= 40 - 18$ $= 22$
Find the number of electrons. The number of electrons is equal to the atomic number because the total negative charge is equal to the total positive charge in an uncharged (neutral) atom.	the number of electrons = $Z = 18$

➤ Try yourself 3.2.1

CALCULATING THE NUMBER OF SUBATOMIC PARTICLES

Calculate the number of protons, neutrons and electrons for the atom with this nuclear symbol:

$^{238}_{92}U$

ISOTOPES

All atoms of the same element have the same number of protons in the nucleus, and therefore the same atomic number, Z. However, not all atoms that belong to the same element have the same mass number, A. For example, hydrogen atoms can have mass numbers of 1, 2 or 3. In other words, hydrogen atoms may contain just a single proton ($A = 1$), a proton and a neutron ($A = 2$), or a proton and two neutrons ($A = 3$), as shown in Figure 3.2.3. Atoms that have the same number of protons (same atomic number) but different numbers of neutrons (and therefore different mass numbers) are known as isotopes. In nature, different elements have different numbers of isotopes. Gold has only one isotope, whereas lead has four isotopes and mercury has seven isotopes.

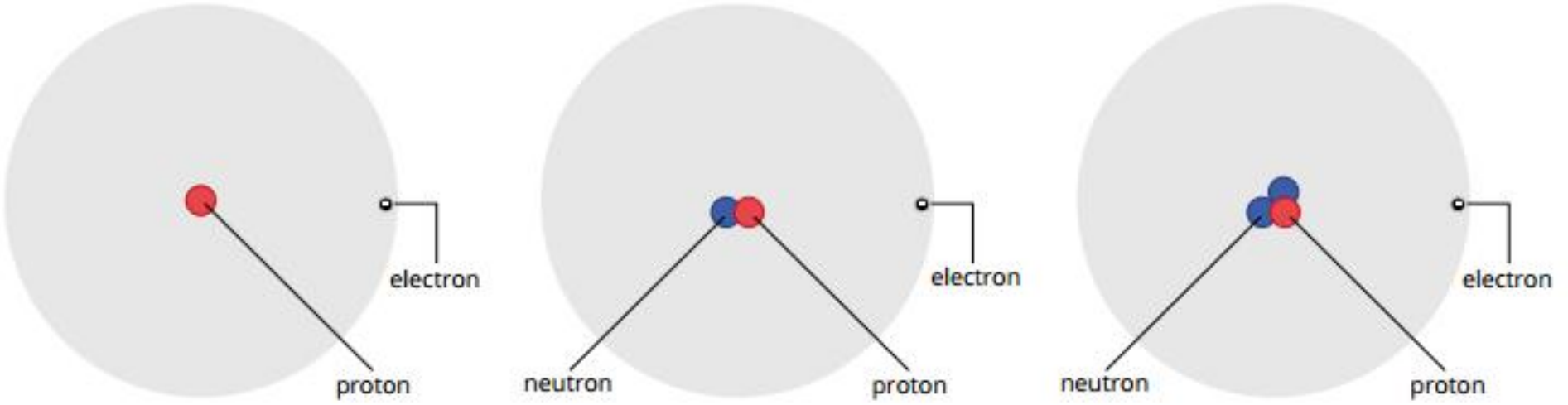


FIGURE 3.2.3 The three isotopes of hydrogen are given special names. A hydrogen atom with just one proton in its nucleus is known as hydrogen or protium. A hydrogen atom with one proton and one neutron is known as deuterium. A hydrogen atom with one proton and two neutrons is known as tritium.

Isotopes have the same arrangements of electrons in the shells of their atoms and their **chemical properties**, such as bonding and chemical reactions, are the same. However, the change in the number of neutrons will alter their mass and density, and their **physical properties** related to mass or density.

The existence of isotopes creates a problem when identifying the atomic mass of an element because each isotope has a different mass. The accepted atomic mass for an element is a **weighted average** of all known isotopes. This is the reason that the atomic masses shown on the periodic table are not whole numbers even though you know atoms have whole numbers of protons and neutrons (each with a mass of 1). Chapter 5 explains this further and describes the calculations that can be used to determine atomic mass.

Carbon has three naturally occurring isotopes, as shown in Figure 3.2.4.

$^{12}_{6}C$	$^{13}_{6}C$	$^{14}_{6}C$
carbon-12	carbon-13	carbon-14

FIGURE 3.2.4 Isotopes of carbon

Nuclear symbol notation is used to identify isotopes because it clearly shows the number of protons and neutrons in each isotope. However, it is common to only show the element symbol or name and its mass number. For example, $^{14}_{6}C$ can be written as ^{14}C or carbon-14.

Carbon-14 and the war against poachers

Isotopes are important in the war against ivory poaching in Africa. All living organisms take up carbon-14 and carbon-12 from the environment to build biologically important structures in the organism. The biochemistry of proteins, DNA, carbohydrates and lipids is based on this crucial element. Over time, the amount of carbon-14 in tissues of plants and animals decreases as the isotope radioactively decays. The levels of carbon-12 remain constant, so the change to the ratio of carbon-14 to carbon-12 (^{14}C:^{12}C) decreases with time. By looking at the levels of the carbon-14 isotope in elephant tusks and ivory, scientists can determine how old the ivory is.

If the authorities know the age of the ivory, then legal action can be taken against the poachers and sellers of the product. Ivory products prior to 1989 are allowed to be traded. Since 1989, the trade in ivory has been made illegal worldwide.

Radioisotopes

Chemists monitor carbon-14 in criminal investigations of poachers. This is one of many examples of the usefulness of these special **radioactive** isotopes, called **radioisotopes**. The forces holding the nucleus of a radioisotope together are unbalanced and over time particles and electromagnetic radiation are emitted from the nucleus. This is measured as **radioactivity**, and was first described by Henri Becquerel, Marie Curie and Pierre Curie in 1903. The three key particles and radiation emitted from radioactive substances (Table 3.2.1) have provided the basis for valuable technologies, but also created health risks to humans. After discovering and characterising the radioactive elements radium and polonium, Marie Curie eventually died from a condition caused by radiation exposure. Even her famous notebooks are too radioactive to be viewed without protection.

TABLE 3.2.1 Three types of radiation: alpha, beta and gamma. Alpha radiation is composed of helium nuclei, beta radiation is composed of electrons and gamma radiation is a form of electromagnetic radiation (from the same spectrum as light, radio waves and microwaves).

Radiation type	Symbol	Identity	Penetrating ability	Examples of sources
alpha	α	helium nucleus, ^4_2He	low	polonium-210 radon-222
beta	β	electron	moderate	carbon-14 sulfur-35
gamma	γ	electromagnetic radiation	high	iodine-125 caesium-137

Radioactive particles and radiation can penetrate matter and interact with biological molecules. The most vulnerable biological structure is the DNA found within the nucleus of almost every cell. Even a change to a single molecule of DNA can alter the way it functions. At the protein level, this may mean that cells divide uncontrollably or do not respond to normal physiological regulation. Some tumours develop in this way. Therefore, safe use of isotopes requires shielding equipment, such as lead panels, to protect the user.

The penetrating ability of radiation emitted by radioisotopes is used in quality control processes to measure the thickness of materials. In smoke detectors, americium-241 (an α emitter) ionises and detects any smoke particles in the air.

Figure 3.2.5 shows the penetrating capabilities of **alpha particles**, and **beta** and **gamma radiation**. These characteristics are used in medical imaging. The image in Figure 3.2.6 was created using a radioactive isotope, in a technique called **positron emission tomography (PET)**.

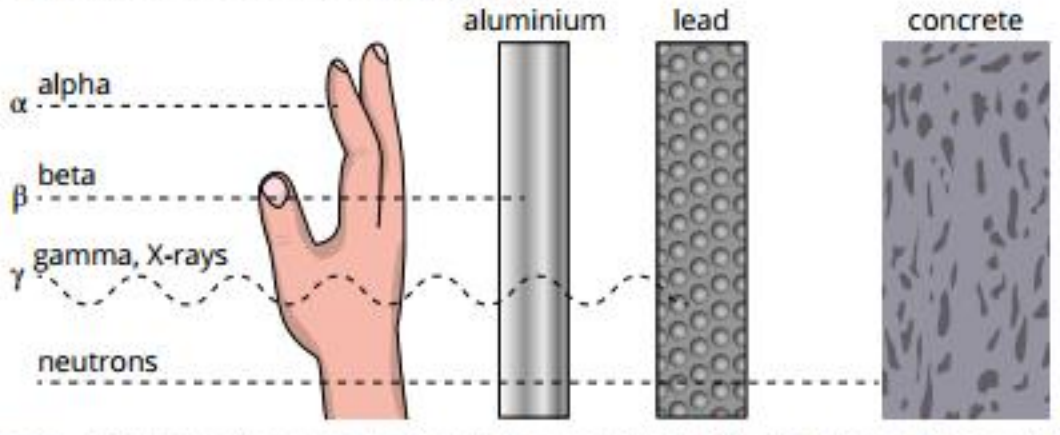


FIGURE 3.2.5 Diagrammatic representation of the penetrating ability of alpha particles, and beta and gamma radiation

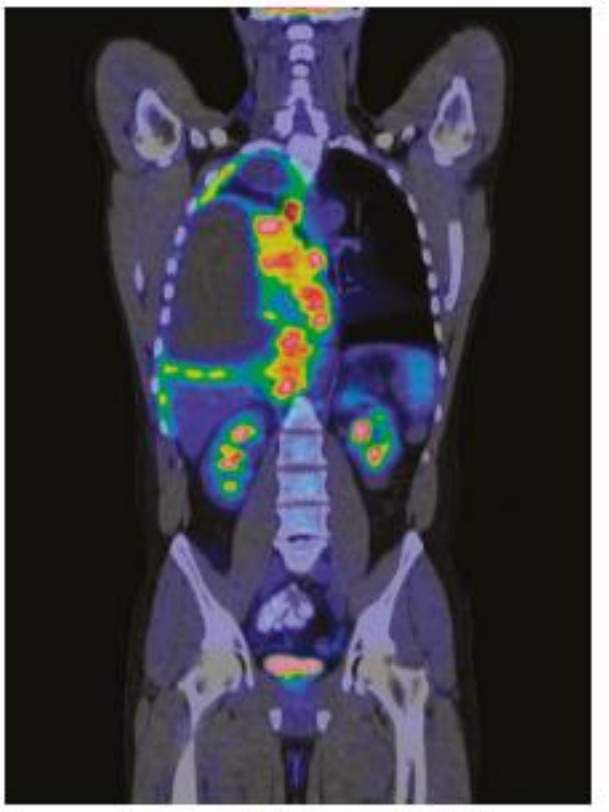


FIGURE 3.2.6 A composite image of a computed tomography (CT) scan and a coloured positron emission tomography (PET) scan of the thorax and abdomen

Radioisotopes have a wide variety of uses, including carbon-14 for carbon dating in geology and palaeobiology; radioactive tracers such as iodine-123 in nuclear medicine; radioimmunoassays for testing constituents of blood, serum, urine, hormones and antigens; and radiotherapy that destroys damaged cells. Use of radioisotopes requires careful evaluation and monitoring because of the potential harmful effects on humans and the environment if their production, use and disposal are not managed effectively. Risks include unwanted damage to cells in the body, especially during pregnancy, and ongoing radiation produced from radioactive sources with long half-lives.

Half-life

The **half-life** of a radioisotope is the time taken for half of the atoms in a sample to decay to a new element or isotope. This can be an extremely short time or millions of years. Figure 3.2.7 shows the number of radioactive particles detected from a sample, measured in counts per second. After two days, the number of particles detected has halved, so the half-life of the particle is two days. By determining the rate of decay (gradient of the graph) at a certain point in time, the age of the specimen can be determined.

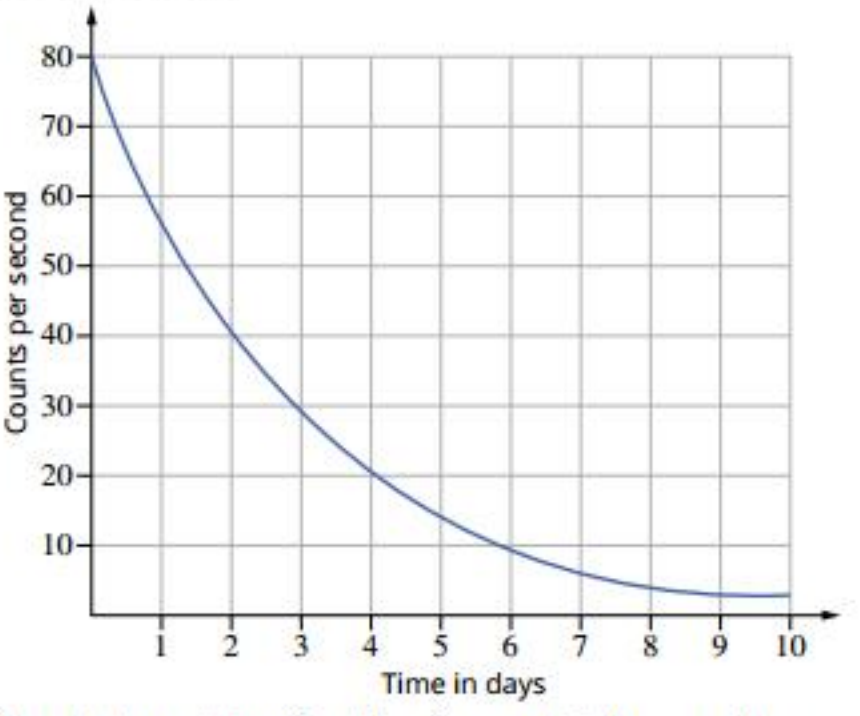


FIGURE 3.2.7 Change in the emission of radiation from a radioisotope over time

Ions

Nuclear symbol notation can also be used to represent **ions**. Ions are atoms that have lost or gained one or more electrons. An atom that loses electrons becomes positively charged (as the positively charged protons in the nucleus outnumber the negatively charged electrons in the cloud). Similarly, an atom that gains electrons becomes negatively charged. You will learn more about ions in Chapter 7.

When an atom gains or loses one or more electrons, it becomes an ion. An ion is a charged particle. Atoms that lose electrons become positive ions. Atoms that gain electrons become negative ions.

Worked example 3.2.2

CALCULATING THE NUMBER OF SUBATOMIC PARTICLES IN AN ION

Calculate the number of protons, neutrons and electrons for the ion with this nuclear symbol:

$^{25}_{12}Mg^{2+}$

Thinking	Working
The atomic number is equal to the number of protons.	the number of protons = Z = 12
Find the number of neutrons. Number of neutrons = mass number − atomic number	the number of neutrons = $A - Z$ = 25 − 12 = 13
Find the number of electrons in an uncharged (neutral) atom. The number of electrons is equal to the atomic number.	the number of electrons in an uncharged (neutral) atom = Z = 12
Find the number of electrons in the ion. The atom has a charge of 2+, which means that it has two fewer electrons than an uncharged atom. Note that this is equal to the atomic number minus the overall charge (Z − charge).	the number of electrons in the ion = 12 − 2 = 10

➤ Try yourself 3.2.2

CALCULATING THE NUMBER OF SUBATOMIC PARTICLES IN AN ION

Calculate the number of protons, neutrons and electrons for the ion with this nuclear symbol:

$^{14}_{7}N^{-}$

3.2 Review

SUMMARY

- Nuclear symbol notation is a way to descriptively write the symbol for an atom together with the atomic number and mass number.
- The number of subatomic particles in an atom can be determined from an element's atomic number and mass number.
- The atomic number indicates how many protons or electrons a neutral (uncharged) atom has.
- The mass number tells you how many protons and neutrons are in the nucleus of an atom. When the atomic number is subtracted from the mass number, the number of neutrons is obtained.
  mass number (A) − atomic number (Z)
- Ions are atoms that have lost or gained electrons to become charged particles.
- Isotopes are atoms with the same atomic number but different mass numbers, i.e. they have the same number of protons but different numbers of neutrons.
- Isotopes have the same chemical properties as other isotopes of the same element but different physical properties, such as mass, density and radioactivity.
- The penetrating ability of radiation from unstable isotope nuclei has uses in our society, but also poses some risks.

KEY QUESTIONS

Describe

1 What do the letters A and Z refer to in the nuclear symbol notation for an isotope ${}^{A}_{Z}X$?

2 How many protons, neutrons and electrons are present in the uncharged atom ${}^{31}_{15}P$?

3 Which element contains seven protons and seven neutrons? Write its nuclear symbol notation.

4 Write the nuclear symbol notation of the following isotopes.
- **a** potassium-39
- **b** nickel-59
- **c** boron-11
- **d** lithium-7

5 Identify these atoms and determine the number of neutrons that each contains.
- **a** ${}^{27}_{13}X$
- **b** ${}^{19}_{9}X$

8 Use the periodic table on page 10 to complete the following table.

Element	Nuclear symbol notation	Atomic number	Mass number	Number of protons	Number of neutrons	Number of electrons
hydrogen				1	0	
hydrogen	${}^{2}_{1}H$					
fluorine		9	19			
sulfur				16	17	
		16	34			
					36	29
	${}^{16}_{8}O$					
				29	34	

Apply

6 Which of the following symbols represent isotopes of the same element?

${}^{14}_{6}X$ ${}^{14}_{7}Y$ ${}^{12}_{6}Z$

7 Explain the similarities and differences between isotopes of the same element.

Analyse

9 Are any of the atoms in the table above isotopes of each other? Explain your reasoning.

10 How many electrons would the ion ${}^{65}_{30}Zn^{2+}$ contain?

11 How many electrons would the ion ${}^{19}_{9}F^{-}$ contain?

12 Suggest why it might be easier to separate ${}^{46}_{20}Ca$ and ${}^{46}_{22}Ti$ than to separate ${}^{46}_{20}Ca$ and ${}^{40}_{20}Ca$.

3.3 Electronic structure of the atom

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that the quantum mechanical model of the atom describes electrons residing in shells, subshells and orbitals
- understand that the location of electrons within atoms in their ground state can be represented using electron configurations indicating the shell, subshell and number of electrons
- understand the relative energies of the *s*, *p* and *d* subshells and the required order of filling of shells and subshells
- understand that the order of filling of subshells is different to the order of writing subshells in an electron configuration
- write electron configurations for atoms and ions up to $Z = 36$ using both full and condensed notation
- use Hund's rule and the Pauli exclusion principle to construct orbital diagrams to represent the relative energy of orbitals for elements up to $Z = 36$
- recognise the electron configurations of Cr and Cu as exceptions.

The shell model of the atom described in Module 3.1 describes electrons as being located in particular energy levels (shells) in an atom. In fact, the electronic structure of an atom appears to be more complicated than this. The model that best explains the experimental findings to date describes electron shells as also containing **subshells**. Scientists, including Erwin Schrödinger, adapted Bohr's model and used mathematics to develop this new model of the atom. The fundamental difference between Bohr's shell model and Schrodinger's model is the way that these models describe the behaviour of electrons. Scientists began to think that electrons inside atoms have wave-like properties and behave very differently from the particles we experience in everyday life. This model of the atom is known as the **quantum mechanical model**.

SHELLS AND SUBSHELLS

The quantum mechanical model describes shells and subshells in the following ways.

- There are major energy levels in an atom that are called shells. The shells (n) are numbered 1, 2, 3, 4, 5, 6 or 7.
- The maximum number of electrons in a shell is $2n^2$.
- The shells contain separate levels of similar energy, called subshells, which are labelled *s*, *p*, *d* and *f*. Each subshell can only hold a certain number of electrons.
- *s* subshells hold two electrons, *p* subshells hold six electrons, *d* subshells hold 10 electrons and *f* subshells hold 14 electrons.

Electrons therefore exist within subshells, which themselves are located within shells. The subshells for the first three shells are summarised in Table 3.3.1. It shows that for the first shell ($n = 1$) there is only an *s* subshell holding a maximum of two electrons. However, in the second shell ($n = 2$), there is an *s* subshell and a *p* subshell. These subshells hold two and six electrons, respectively, and so the total number of electrons in the shell is 8. Note that the total number of electrons is still $2n^2$.

TABLE 3.3.1 Subshells for the first three shells

Shell number (n)	Subshells present	Maximum number of electrons in subshell	Name of subshell	Total maximum number of electrons in shell
1	s	2	$1s$	2
2	s p	2 6	$2s$ $2p$	8
3	s p d	2 6 10	$3s$ $3p$ $3d$	18

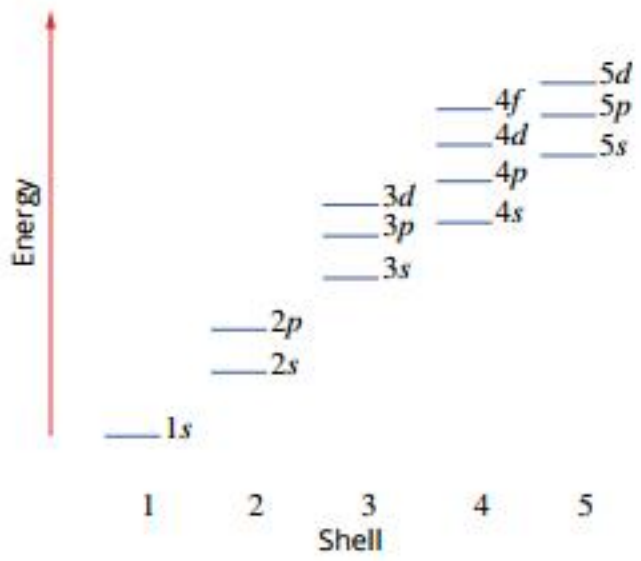


FIGURE 3.3.1 Subshells of the quantum mechanical model and their relative energy levels

The name of each subshell tells us two things—the energy level and the type of subshell. For example, a $3s$ subshell is in the third energy level ($n = 3$) and will hold a maximum of two electrons.

A useful way to represent the quantum mechanical model is to view all of the subshells relative to their energy levels. Remember that the inner shells and subshells are lower in energy. Figure 3.3.1 shows that the outer shells contain more subshells and are higher in energy overall than the inner shells. For example, the $n = 4$ shell contains s, p, d and f subshells, whereas the $n = 2$ shell contains only an s and a p subshell. (Note: the $n = 5$ shell on this diagram is incomplete.)

The order of 'filling' electrons into these shells and subshells starts at the lowest energy subshell in the shell $n = 1$ before filling higher energy subshells. This is known as the **Aufbau principle**. Figure 3.3.1 shows that the subshells increase in energy in the following order: $1s$, $2s$, $2p$, $3s$, $3p$, etc.

Table 3.3.1 and Figure 3.3.1 can be used to determine the number of electrons in each subshell for a given atom.

The Aufbau principle states that for atoms in their lowest energy state, electrons first fill up the lower energy subshells before progressively filling up the higher ones.

Worked example 3.3.1

ELECTRON DISTRIBUTION ACROSS SUBSHELLS

Apply the rules of the quantum mechanical model to determine the number of electrons in each subshell of a neon atom with 10 electrons.

Thinking	Working
Recall the maximum number of electrons that each (s, p, d or f) subshell can hold.	subshell — maximum number of electrons s — 2 p — 6 d — 10 f — 14
Recall the order of filling of subshells.	$1s > 2s > 2p > 3s > 3p$...
Start at the first subshell and place the correct number of electrons in the subshells from the lowest energy to the highest energy. Do not exceed the maximum number of electrons allowed.	subshell — electrons $1s$ — 2 $2s$ — 2 $2p$ — 6
Write the number of electrons in each subshell.	This atom has two electrons in the $1s$ subshell, two electrons in the $2s$ subshell and six electrons in the $2p$ subshell.

➤ Try yourself 3.3.1

ELECTRON DISTRIBUTION ACROSS SUBSHELLS

Apply the rules of the quantum mechanical model to determine the number of electrons in each subshell of an atom with 13 electrons.

ELECTRON DISTRIBUTION FOR ATOMS WITH MORE THAN 18 ELECTRONS

Look closely at the section of Figure 3.3.1 where the subshells in the third ($n = 3$) and the fourth ($n = 4$) shells are shown. The energy level of 4*s* is *below* that of 3*d*. This means that the 4*s* subshell will fill before the third shell is completely full. Also, some subshells in the fifth energy level will fill before the fourth shell is complete. This means that the quantum mechanical order of filling does not simply complete each shell in turn, but fills part of two shells at the same time.

The order of filling of subshells is
1*s* > 2*s* > 2*p* > 3*s* > 3*p* > 4*s* > 3*d* > 4*p* > 5*s* > 4*d* > 5*p*...

So, to find the arrangement of electrons in atoms with more than 18 electrons, you follow the same procedure, being careful to identify the subshell with the next lowest energy level. The first two electrons fill the 1*s* subshell in the first shell. The next eight electrons fill the *s* and *p* subshells in the second shell. The next eight electrons fill the *s* and *p* subshells in the third shell. The 4*s* subshell is then filled with two electrons because this subshell is lower in energy than the 3*d* subshell. Once the 4*s* subshell is filled, the next 10 electrons are placed in the 3*d* subshell, followed by the 4*p* subshell.

The geometric pattern shown in Figure 3.3.2 is a convenient way of remembering the order in which the subshells are filled. The electron arrangements of chromium and copper atoms are exceptions to the rule (see page 43).

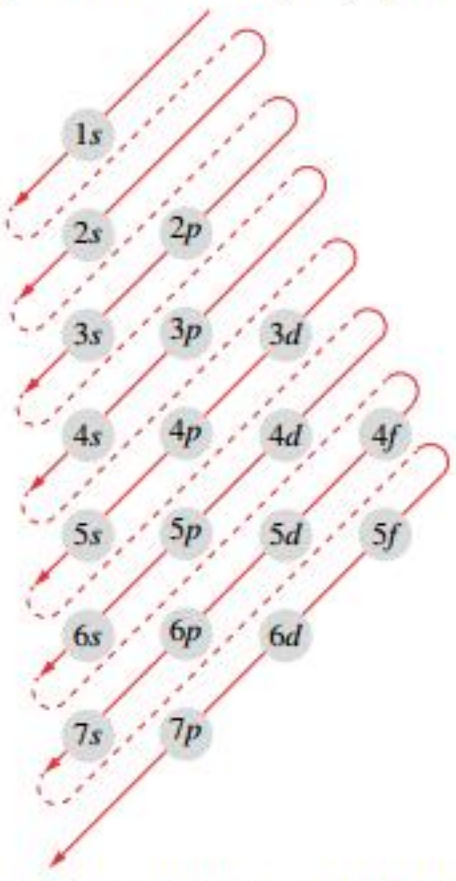


FIGURE 3.3.2 This geometric pattern shows the order in which the subshells are filled. Note that the fourth shell starts filling before the third shell is completely filled. This is because the 4*s* subshell is lower in energy than the 3*d* subshell. As a result, the 4*s* subshell accepts two electrons after the 3*s* and 3*p* subshells are filled, but before the 3*d* subshell begins filling.

WRITING ELECTRON CONFIGURATIONS USING SUBSHELL DESIGNATIONS

When writing the **electron configuration** (arrangement of electrons) of an atom based on the quantum mechanical model, the number of electrons in each subshell must be shown. For example, the electron configuration of a sodium atom is shown in Figure 3.3.3.

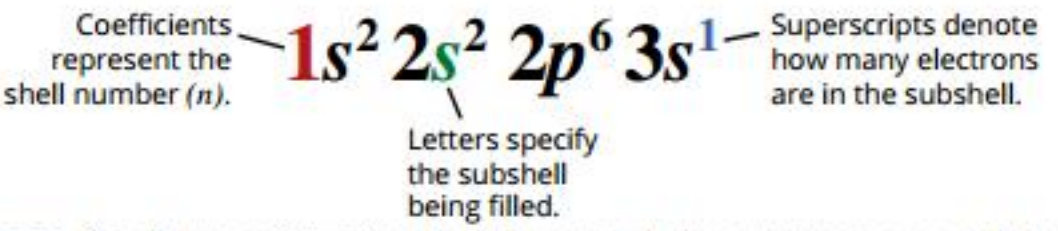

Coefficients represent the shell number (n).
1s² 2s² 2p⁶ 3s¹
Superscripts denote how many electrons are in the subshell.
Letters specify the subshell being filled.

FIGURE 3.3.3 The electron configuration of a sodium atom. It shows that there are two electrons in the 1s subshell, two electrons in the 2s subshell, six electrons in the 2p subshell and one electron in the 3s subshell. Note that the total number of electrons in the atom can be obtained by adding the superscripts.

Krypton has 36 electrons. According to the quantum mechanical order of subshell filling, its configuration is:

$$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6$$

Although the 4*s* subshell is filled before the 3*d* subshell, the subshells of the third shell are usually grouped together. Therefore, the electron configuration for a krypton atom is written as:

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$$

This means that after you have used the order of filling and written the electron configuration, it needs to be rewritten so that the subshells with the same *n* value are grouped together, as shown in Figure 3.3.4.

$$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$$

FIGURE 3.3.4 Electron configuration of krypton showing the grouping of subshells with the same *n* value

Worked example 3.3.2

WRITING ELECTRON CONFIGURATIONS USING SUBSHELL DESIGNATIONS

Apply the rules of the quantum mechanical model to write the electron configuration of a strontium atom with 38 electrons.	
Thinking	**Working**
Recall the maximum number of electrons that each (*s*, *p*, *d* or *f*) subshell can hold.	subshell — maximum number of electrons *s* — 2 *p* — 6 *d* — 10 *f* — 14
Recall the order of filling of subshells.	1*s* > 2*s* > 2*p* > 3*s* > 3*p* > 4*s* > 3*d* > 4*p* > 5*s*...
Start at the first subshell and place the correct number of electrons in the subshells from the lowest energy to the highest energy. Do not exceed the maximum number of electrons allowed per subshell.	subshell — electrons 1*s* — 2 2*s* — 2 2*p* — 6 3*s* — 2 3*p* — 6 4*s* — 2 3*d* — 10 4*p* — 6 5*s* — 2

Write the electron configuration of strontium by placing the electron number as a superscript to each subshell.	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2$
Rewrite the electron configuration, grouping subshells from the same shell together.	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 5s^2$

➤ Try yourself 3.3.2

WRITING ELECTRON CONFIGURATIONS USING SUBSHELL DESIGNATIONS

Apply the rules of the quantum mechanical model to write the electron configuration of an arsenic atom with 33 electrons.

Writing condensed electron configurations

An electron configuration is sometimes written in shorthand as a **condensed electron configuration** (also called **noble gas notation)**. The condensed electron configuration of an element starts with the symbol for the noble gas (in square brackets) in the period before the element in the periodic table. This means that the electron configuration for the inner shells is not written—it is implied by the use of the noble gas symbol.

For example, the condensed electron configuration of phosphorus ($1s^2 2s^2 2p^6 3s^2 3p^3$) is [Ne]$3s^2 3p^3$. The [Ne] symbol signifies $1s^2 2s^2 2p^6$ because this is the electron configuration of neon. Some other examples of condensed electron configurations are shown in Table 3.3.2. This abbreviation of the full **electron configuration notation** is especially useful for elements with multiple shells containing electrons.

Both ways of writing electron configurations are correct. However, an advantage of the condensed notation is that the number of valence electrons (electrons in the outermost shell) is clear. As we will see in later chapters, this number is fundamental to describing how the atom bonds with other atoms.

TABLE 3.3.2 Some examples of the use of condensed electron configuration

Element	Atomic number	Electron configuration	Condensed electron configuration
Si	14	$1s^2 2s^2 2p^6 3s^2 3p^2$	[Ne]$3s^2 3p^2$
Zn	30	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$	[Ar]$3d^{10} 4s^2$
Br	35	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$	[Ar]$3d^{10} 4s^2 4p^5$

Worked example 3.3.3

WRITING CONDENSED ELECTRON CONFIGURATIONS FOR UP TO 36 ELECTRONS

Write the condensed electron configuration of a silicon atom with 14 electrons.

Thinking

Recall the maximum number of electrons that each (*s*, *p*, *d* or *f*) subshell can hold.

Working

subshell	maximum number of electrons
s	2
p	6
d	10
f	14

Recall the order of filling of subshells.	$1s > 2s > 2p > 3s > 3p > 4s > 3d > 4p > 5s$...
Start at the first subshell and place the correct number of electrons in the subshells from the lowest energy to the highest energy. Do not exceed the maximum number of electrons allowed per subshell.	subshell — electrons $1s$ — 2 $2s$ — 2 $2p$ — 6 $3s$ — 2 $3p$ — 2
Write the full electron configuration of silicon by placing the electron number as a superscript to each subshell. If necessary, rewrite the electron configuration, grouping subshells from the same shell together.	$1s^2 2s^2 2p^6 3s^2 3p^2$
Identify the noble gas in the period before silicon and replace its electron configuration with its element symbol in square brackets.	The noble gas before silicon is neon. $[Ne]3s^2 3p^2$

➤ Try yourself 3.3.3

WRITING CONDENSED ELECTRON CONFIGURATIONS FOR UP TO 36 ELECTRONS

Write the condensed electron configuration of a calcium atom with 20 electrons.

Writing electron configurations using condensed notation clearly shows the number of valence electrons, as shown in Table 3.3.3.

TABLE 3.3.3 Examples of electron configurations using condensed notation

Z	Element		Configuration	Z	Element		Configuration
1	H	hydrogen	$1s^1$	18	Ar	argon	$[Ne]3s^2 3p^6$
2	He	helium	$1s^2$	19	K	potassium	$[Ar]4s^1$
3	Li	lithium	$[He]2s^1$	21	Sc	scandium	$[Ar]3d^1 4s^2$
4	Be	beryllium	$[He]2s^2$	22	Ti	titanium	$[Ar]3d^2 4s^2$
5	B	boron	$[He]2s^2 2p^1$	24	Cr	chromium	$[Ar]3d^5 4s^1$
6	C	carbon	$[He]2s^2 2p^2$	26	Fe	iron	$[Ar]3d^6 4s^2$
9	F	fluorine	$[He]2s^2 2p^5$	28	Ni	nickel	$[Ar]3d^8 4s^2$
10	Ne	neon	$[He]2s^2 2p^6$	29	Cu	copper	$[Ar]3d^{10} 4s^1$
11	Na	sodium	$[Ne]3s^1$	30	Zn	zinc	$[Ar]3d^{10} 4s^2$
12	Mg	magnesium	$[Ne]3s^2$	31	Ga	gallium	$[Ar]3d^{10} 4s^2 4p^1$
13	Al	aluminium	$[Ne]3s^2 3p^1$	35	Br	bromine	$[Ar]3d^{10} 4s^2 4p^5$
17	Cl	chlorine	$[Ne]3s^2 3p^5$	36	Kr	krypton	$[Ar]3d^{10} 4s^2 4p^6$

Chromium and copper—exceptions

The electron configurations for most elements follow the rules described above. There are two notable exceptions: chromium ($Z = 24$) and copper ($Z = 29$). Table 3.3.4 shows their electron configurations.

TABLE 3.3.4 The electron configurations for chromium and copper

Element	Electron configuration predicted using the rules above	Actual electron configuration
chromium, Cr	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^4 4s^2$	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^1$
copper, Cu	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 4s^2$	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$

Chemists calculate that there is little difference in energy between the $3d$ and $4s$ subshells, and the $3d^5 4s^1$ configuration for chromium is slightly more stable than the $3d^4 4s^2$ configuration. This occurs when the $3d$ subshell is exactly half-filled.

Similarly, for copper, the $3d^{10} 4s^1$ arrangement with a completely filled $3d$ subshell and an incompletely filled s subshell provides additional stability compared to the filled s subshell and incompletely filled d subshell.

ORBITALS AND ORBITAL DIAGRAMS

The quantum mechanical model proposes that each subshell in an atom is made up of smaller components known as **orbitals**. Orbitals can hold up to two electrons and can be described as regions of space surrounding the nucleus of an atom in which electrons may be found. An s subshell has just one orbital, a p subshell has three orbitals, a d subshell has five orbitals and an f subshell has seven orbitals. In diagrammatic representations of electron configurations, the symbol ⇅ can be used to indicate two electrons in an orbital.

i Orbitals can be described as regions of space surrounding the nucleus of an atom in which electrons may be found. An s subshell has one orbital, a p subshell has three orbitals, a d subshell has five orbitals and an f subshell has seven orbitals.

An **orbital diagram** shows each of the separate orbitals occupied by electrons in an atom and helps to correctly determine the electron configuration of the atom. For example, neon has 10 electrons and so will have both its first and second shells full. The subshells that have been filled are $1s$, $2s$ and $2p$. The first two electrons fill the $1s$ subshell, the second two electrons go into the next highest energy level, the $2s$ subshell, and the last six electrons then fill the next highest energy level, the $2p$ subshell. The electron configuration is written as $1s^2 2s^2 2p^6$, and the orbital diagram is shown in Figure 3.3.5. In this diagram, each box represents an orbital that can hold two electrons.

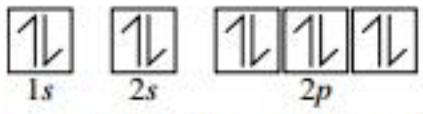


FIGURE 3.3.5 Orbital diagram showing the electron configuration of neon, also written as $1s^2 2s^2 2p^6$. Each box represents an orbital and each arrow represents an electron.

Electrons have a characteristic known as electron spin, which can take one of two orientations: 'spin up' or 'spin down'. The arrows in the orbital diagram represent these two orientations. This gives rise to the **Pauli exclusion principle** in the quantum mechanical model of the atom, which in essence states that no more than two electrons can occupy the same orbital and they must have opposite spin.

i The Pauli exclusion principle indicates that no more than two electrons can be in one orbital, and they must have opposite spin (as shown by arrows).

The orbital diagram in Figure 3.3.5 shows how the 10 electrons in a neon atom are distributed across the orbitals in the $1s$, $2s$ and $2p$ subshells. Figure 3.3.6 shows a slightly different way to represent orbital diagrams, ranking the order of the energies of the subshells. Known as an orbital energy level diagram, this type of diagram shows the relative energies of electrons distributed across the orbitals, subshells and shells. Both orbital diagram representations are valid and convey slightly different information about electron configuration.

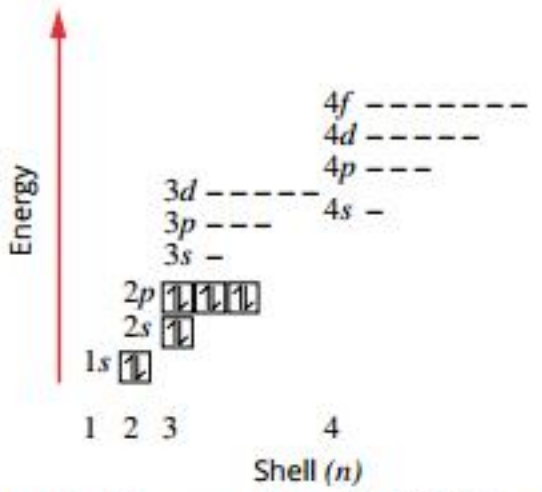


FIGURE 3.3.6 This orbital energy level diagram of neon ($1s^2 2s^2 2p^6$) shows the relative energies of electrons in orbitals distributed across the 1*s*, 2*s* and 2*p* subshells.

The orbital diagrams for neon in Figures 3.3.5 and 3.3.6 above have the 1*s*, 2*s* and 2*p* subshells full. **Hund's rule** describes how to arrange electrons in other cases when a *p* or *d* subshell is not full. Hund's rule states that every orbital in a subshell is singly occupied (each contains one electron with the same spin) before any orbital is doubly occupied (contains two electrons, the second one with the opposite spin). Figure 3.3.7 shows how this works in practice. Nitrogen has three electrons in the 2*p* subshell and these occupy separate orbitals. As the atomic number increases (from N to Ne), the 2*p* subshell becomes progressively filled.

Hund's rule states that orbitals of equal energy are each occupied by one electron before any orbital is occupied by a second electron.

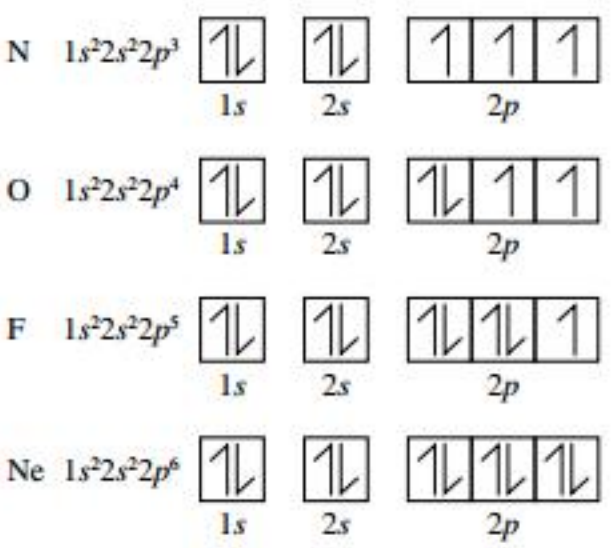


FIGURE 3.3.7 Electron configurations of nitrogen (N), oxygen (O), fluorine (F) and neon (Ne) showing the application of Hund's rule. In the case of nitrogen, it has three electrons with the same spin in separate 2*p* orbitals.

3.3 Review

SUMMARY

- The quantum mechanical model proposes that electrons in atoms are grouped in shells, subshells and orbitals, as shown in the table below.

Shell	Subshells	Orbitals in subshell
1	1*s*	1
2	2*s* 2*p*	1 3
3	3*s* 3*p* 3*d*	1 3 5
4	4*s* 4*p* 4*d* 4*f*	1 3 5 7

- An orbital can be described as a region of space surrounding the nucleus of an atom where electrons can be found.
- A subshell consists of orbitals of the same energy; they are represented by the letters *s*, *p*, *d* and *f*.
- An orbital diagram shows each orbital as a box containing up to two electrons (shown as arrows pointing in opposite directions).
- The 4*s* subshell is lower in energy than the 3*d* subshell, so the fourth shell can accept two electrons before the third shell is filled.
- A consequence of the Pauli exclusion principle is that no more than two electrons can occupy the same orbital in an atom.
- The Aufbau principle states that subshells of lower energy will be filled before higher energy subshells.
- The order of filling of subshells is $1s > 2s > 2p > 3s > 3p > 4s > 3d > 4p\ldots$; however, the order of writing the electron configuration is $1s2s3s3p3d4s4p\ldots$
- Cr and Cu are exceptions to the order of filling because their 4*s* subshell is not filled before the 3*d* subshell accepts electrons.
- Electron configurations specify the number of electrons in each subshell using a superscript, e.g. $1s^22s^22p^63s^23p^63d^{10}4s^24p^6$.
- Hund's rule states that every orbital in a subshell is singly occupied (with electrons that have the same spin) before any orbital is doubly occupied (with a second electron that has the opposite spin).
- A condensed electron configuration uses the element symbol for the noble gas that occurs before the element in the periodic table. This symbol is written in square brackets and represents the electron configuration of the noble gas. For example, the condensed electron configuration of boron is $[He]2s^22p^1$.

KEY QUESTIONS

Describe

1 Recall the number of electrons that can be held in each of the subshell types (*s*, *p*, *d* and *f*). Complete the table by using colour coding or drawing lines to identify the maximum number of electrons in each shell.

Subshell	Electron number
s	14
p	2
d	10
f	6

2 Consider the subshells 3*d*, 4*s*, 3*p* and 3*s*.

a Which one has the lowest energy?

b Which one has the highest energy?

3 Refer to Figure 3.3.1. Write the order of filling of electron subshells from 1*s* to 5*s*.

3.3 Review *continued*

4 Write the electron arrangements and the full electron configuration notation for each of the atoms listed in the following table. The first row (boron) has been completed for you as an example.

Element (atomic number)	Arrangement of electrons in shells (shell model)	Electron configuration using the quantum mechanical model
boron (5)	2,3	$1s^2 2s^2 2p^1$
lithium (3)		
chlorine (17)		
sodium (11)		
neon (10)		
potassium (19)		
scandium (21)		
iron (26)		
bromine (35)		

Apply

5 Draw the orbital diagrams for Cl, Be, C, Mn and P.

6 Write the electron configuration of Fe, which has 26 electrons. (You may find Figure 3.3.2 useful for answering this question.)

7 Write the condensed electron configurations for the following elements.

a Ca

b Na

c Cl

8 The condensed electron configuration of a silicon atom is $[Ne]3s^2 3p^2$.

a Write the full electron configuration.

b How many valence electrons does a silicon atom have?

9 Describe the essential difference between the shell model and the quantum mechanical model of the atom in terms of energy levels.

10 Three students incorrectly wrote the following electron configurations. Explain the error in each one.

a $1s^2 2s^1 2p^4$

b $1s^2 2s^2 2p^6 3p^6$

c $1s^3 2s^2 2p^6 3s^2$

11 Why are the electron configurations of copper and chromium exceptions to the rules for electron configurations?

Analyse

12 Identify the elements shown by the following electron configurations.

a $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$

b $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5 4s^2$

c $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^2$

13 Identify the elements shown by the following condensed electron configurations.

a $[Kr]4d^{10} 5s^2 5p^3$

b $[Kr]4d^{10} 5s^2 5p^6$

c $[Ar]4s^1$

14 Three students wrote the following electron configurations for an oxygen atom.

I $1s^2 2s^2 2p^4$

II $1s^4 2s^4$

III $1s^2 2s^2 3s^2 3p^2$

Which electron configuration is correct? Explain why the other configurations are incorrect, referring to the Aufbau principle and the Pauli exclusion principle.

Chapter review

03

KEY TERMS

alpha particle
atom
atomic number
Aufbau principle
beta radiation
Bohr diagram
Bohr model
chemical property
condensed electron configuration
electron
electron configuration
electron configuration notation
electron shell
electrostatic attraction
element
emission spectrum
energy level
excited state
gamma radiation
ground state
half-life
Hund's rule
ion
ionisation energy
isotope
mass number
matter
neutron
noble gas notation
nuclear symbol notation
nucleon
nucleus
octet rule
orbital
orbital diagram
Pauli exclusion principle
periodic table (of elements)
physical property
positron emission tomography (PET)
proton
quanta
quantum mechanical model
radioactive
radioactivity
radioisotope
scientific model
shell model
subatomic particle
subshell
valence electron
valence shell
weighted average

KEY QUESTIONS

Describe

1 Compare the mass and charge of protons, neutrons and electrons.

2 Which of the following lists the maximum number of electrons in the first three shells of an atom?

A 8,8,18
B 2,8,12
C 2,8,8
D 2,8,18

3 Isotopes of an element contain different numbers of:

A protons and electrons
B neutrons and nucleons
C nucleons and electrons
D electrons and neutrons.

4 Which one of the following correctly defines the mass number of an atom?

A the total number of neutrons and protons in the nucleus of the atom
B the number of protons in the nucleus of the atom
C the total mass of neutrons and protons in the nucleus of the atom
D the total mass of the atom

5 Identify which of the following atoms are not in their lowest energy state. Recall that electrons can 'jump' to a higher energy level (excited state) when they are heated and then release light energy as they return to their lower energy level (ground state).

A $1s^2 2s^2 2p^6 3s^1$
B $1s^2 2s^2 2p^6 3s^2 3p^6$
C $1s^2 2s^2 2p^6 3s^2 3p^5 4s^2$
D $1s^2 2s^2 2p^3$

6 Where would you find 99.97% of the mass of an atom?

7 How are protons, neutrons and electrons arranged in an atom?

8 An atom of chromium can be represented by the symbol $^{52}_{24}Cr$.

a State the atomic number and mass number for chromium.
b Identify the number of electrons, protons and neutrons in the chromium atom.

9 Write the nuclear symbol notation for each isotope.

a phosphorus-31
b bromine-80
c beryllium-9
d gallium-70

10 Write the name and symbol of the element that has each of these electron configurations in its shells.

a 2,7
b 2,8,18,1
c 2,8,5
d 2,8,18,16,1

11 Write electron configurations, using subshell designations, for the following elements. The atomic number of each element is shown in brackets.

a helium (2)
b carbon (6)
c aluminium (13)
d nickel (28)

12 How many orbitals are there in the 2*p* subshell of an atom?
- **A** 2
- **B** 3
- **C** 5
- **D** 6

13 Identify the elements shown by the following electron configurations.
- **a** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^1$
- **b** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$
- **c** $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
- **d** $1s^2 2s^2 2p^6 3s^2 3p^5$

14 Identify the following elements.
- **a** $[Ne]3s^1$
- **b** $[Ne]3s^2 3p^1$
- **c** $[Ar]3d^3 4s^2$
- **d** $[Ar]3d^{10} 4s^2 4p^1$

Apply

15 Determine the number of valence electrons for an atom with 10 electrons. Draw a Bohr diagram for this atom.

16 The nucleus of an atom has a radius of the order of 10^{-13} cm and the atom has a radius of the order of 10^{-9} cm. If the nucleus could be scaled up to the size of an orange (radius 10 cm), what would be the radius of the atom on that same scale?

17 Explain the rule describing the maximum number of electrons in each shell.

18 Determine what element these nuclear symbols represent and calculate the number of neutrons each contains.
- **a** ${}^{119}_{50}X$
- **b** ${}^{23}_{11}X$
- **c** ${}^{96}_{42}X$
- **d** ${}^{27}_{13}X$

19 Explain why the number of electrons in an atom equals the number of protons.

20 How many electrons would the following ions contain?
- **a** ${}^{35}_{17}Cl^-$
- **b** ${}^{238}_{92}U^{2+}$
- **c** ${}^{2}_{1}H^+$
- **d** ${}^{32}_{16}S^{2-}$

21 A bromide ion is composed of 36 electrons, 35 protons and 45 neutrons. The ion is represented by the symbol:
- **A** ${}^{36}_{35}Br^-$
- **B** ${}^{80}_{35}Br^+$
- **C** ${}^{80}_{35}Br^-$
- **D** ${}^{36}_{35}Br^+$.

22 ${}^{37}Cl$ and ${}^{35}Cl$ are regarded as the same element because:
- **A** their atoms have the same mass number
- **B** their atomic numbers differ
- **C** their atoms have similar properties
- **D** their atoms have 17 protons in their nuclei.

23 Using the element carbon as an example, explain why elements are best identified by their atomic number and not their mass number.

24 Write the electron configuration based on the quantum mechanical model for an atom with the following arrangement of electrons in its shells: 2,8,14,2.

25 Which shell and subshell would the 30th electron of an atom go into, according to the rules for determining the electron configuration of an atom?

Analyse

26 Two atoms both have 10 neutrons in their nucleus. The first has 9 protons and the other has 10 protons. Are they isotopes of the same element? Explain your answer.

27 Analyse the following list of atoms.

${}^{27}_{13}A$ ${}^{40}_{20}B$ ${}^{32}_{16}C$ ${}^{14}_{7}D$ ${}^{8}_{3}E$ ${}^{15}_{7}F$ ${}^{19}_{9}G$ ${}^{20}_{9}H$ ${}^{4}_{2}I$
- **a** Which pairs of atoms are isotopes of the same element?
- **b** Which atoms have equal numbers of protons and neutrons in their nuclei?
- **c** Which atom is an isotope of sulfur?
- **d** Which atom has one more electron than a magnesium atom?
- **e** How many different elements are shown?

28 Describe the difference between shells, subshells and orbitals using a fluorine atom as an example.

29 Four sets of atoms and ions are listed below. In which set do all of the atoms and ions have the same number of electrons in the valence shell?
- **A** Li, C, B, Be
- **B** Ca^{2+}, Ne, K^+, Cl^-
- **C** K^+, Cs^+, Na^+, Li^+
- **D** F^-, O^{2-}, Na^+, Ne

30 Why is the 4*s* subshell in chromium and copper only half-filled before the 3*d* subshell begins to be filled?

31 Consider the ionisation energy graph for sodium in Figure 3.1.7 on page 28. Sketch a similar graph for boron that shows the loss of each of its five electrons.

Interpret

32 Determine the electron configuration of a barium atom. Write the arrangement of electrons in this atom using:
- **a** full electron configuration notation
- **b** condensed electron configuration notation.

CHAPTER

04 The periodic table and periodic trends

The periodic table is an organisational tool to describe and explain trends in the structures and properties of the elements within the groups and periods of the table. In particular, you will look at the trends in characteristics and properties of the elements, such as their electron configuration, atomic size, ionic size, first ionisation energy and electronegativity as well as their behaviour as metals or non-metals, and their reactivity. In addition, you will understand the relationship between valence electrons and electrostatic attractions, where electrons are lost, gained or shared to form chemical bonds.

Syllabus subject matter

Topic 1 • Properties and structure of atoms

■ PERIODIC TABLE AND TRENDS

- State that elements are represented by symbols. **4.1**
- Identify that the structure of the periodic table is based on increasing atomic number. **4.1**
- Identify that the periodic table is arranged into four blocks associated with the four sub-levels—*s*, *p*, *d* and *f*. **4.1**
- Describe the relationship between the structure of the periodic table and the electronic configuration of atoms. **4.1**
- Explain that elements of the periodic table show trends in chemical and physical properties across periods and down groups as exemplified by groups 1, 2, 13–18 and period 3. **4.2**
- Compare the metallic and non-metallic behaviours of elements, including group trends and the reactivity for the alkali metals (Li–Cs) and the halogens (F–I). **4.3**
- Identify that oxides change from basic through amphoteric to acidic across period 3. **4.3**
- Analyse data for atomic radii, valencies, ionic radii, 1st ionisation energy and electronegativities to determine periodic trends, patterns and relationships. **4.3**

■ INTRODUCTION TO BONDING

- Explain that the ability of atoms to form chemical bonds is related to the arrangement of electrons in the atom and the stability of the valence electron shell. **4.4**
- Identify that the number of electrons lost, gained or shared is determined by the electron configuration of the atom. **4.4**
- Explain that ions are atoms or groups of atoms that are electrically charged due to an imbalance in the number of electrons and protons. **4.4**
- Explain that chemical bonds are caused by electrostatic attractions that arise because of the sharing or transfer of electrons. **4.4**

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4.1 The periodic table

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- recognise that elements are categorised into groups, periods and blocks within the periodic table based on their electron configuration
- determine the number of valence electrons of an element based on its group
- determine the period of an element based on the number of occupied shells
- identify the period and group of an element based on its electron configuration
- identify an element from its group and period.

Chapter 3 looked at research into elements and the nature of atoms, the existence of subatomic particles, their charge and mass, the way particles are arranged in an atom and the way they behave. As scientists' understanding of the atom improved, and more elements were discovered, a way of organising this knowledge was needed.

The **periodic table** (Figure 4.1.1) is one of the most useful reference tools available to chemists. It minimises the need to memorise isolated facts about different elements and provides a framework for organizing our understanding. By knowing the properties of particular elements and trends within the table, chemists are able to organise what would otherwise be an overwhelming collection of disorganised information.

THE MODERN PERIODIC TABLE

The number of protons (the **atomic number**) is what makes one element fundamentally different from another element. The elements in the modern periodic table are arranged in rows in order of increasing atomic number.

Chemists use the number of electrons in the outermost (valence) shell, called the **valence electrons** (see Chapter 3), to organise the elements into columns. The form of the periodic table in common use is shown in Figure 4.1.1.

KEY: non-metals; metals; metalloids

atomic number — symbol — name: 13 Al aluminium

1 H hydrogen																	2 He helium
3 Li lithium	4 Be beryllium											5 B boron	6 C carbon	7 N nitrogen	8 O oxygen	9 F fluorine	10 Ne neon
11 Na sodium	12 Mg magnesium											13 Al aluminium	14 Si silicon	15 P phosphorus	16 S sulfur	17 Cl chlorine	18 Ar argon
19 K potassium	20 Ca calcium	21 Sc scandium	22 Ti titanium	23 V vanadium	24 Cr chromium	25 Mn manganese	26 Fe iron	27 Co cobalt	28 Ni nickel	29 Cu copper	30 Zn zinc	31 Ga gallium	32 Ge germanium	33 As arsenic	34 Se selenium	35 Br bromine	36 Kr krypton
37 Rb rubidium	38 Sr strontium	39 Y yttrium	40 Zr zirconium	41 Nb niobium	42 Mo molybdenum	43 Tc technetium	44 Ru ruthenium	45 Rh rhodium	46 Pd palladium	47 Ag silver	48 Cd cadmium	49 In indium	50 Sn tin	51 Sb antimony	52 Te tellurium	53 I iodine	54 Xe xenon
55 Cs caesium	56 Ba barium	57–71 lanthanoids	72 Hf hafnium	73 Ta tantalum	74 W tungsten	75 Re rhenium	76 Os osmium	77 Ir iridium	78 Pt platinum	79 Au gold	80 Hg mercury	81 Tl thallium	82 Pb lead	83 Bi bismuth	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89–103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium	113 Nh nihonium	114 Fl flerovium	115 Mc moscovium	116 Lv livermorium	117 Ts tennessine	118 Og oganesson

Lanthanoids	57 La lanthanum	58 Ce cerium	59 Pr praseodymium	60 Nd neodymium	61 Pm promethium	62 Sm samarium	63 Eu europium	64 Gd gadolinium	65 Tb terbium	66 Dy dysprosium	67 Ho holmium	68 Er erbium	69 Tm thulium	70 Yb ytterbium	71 Lu lutetium
Actinoids	89 Ac actinium	90 Th thorium	91 Pa protactinium	92 U uranium	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

FIGURE 4.1.1 The form of the periodic table in common use

The modern periodic table has several key features (numbering is based on the IUPAC convention).

- The periodic table is arranged in order of increasing atomic number.
- The horizontal rows are known as **periods** and are labelled 1–7.
- The vertical columns are known as **groups** and are labelled 1–18.
- **Main group elements** are elements in groups 1, 2 and 13–18.
- The elements in groups 3–12 are known as **transition metals**.

Some periodic tables you will see also indicate other properties of the elements such as boiling point or whether the element is a solid, liquid or gas at room temperature.

The International Union of Pure and Applied Chemistry (IUPAC) is an international organisation of chemists working to advance their science and create common standards and nomenclature (a set of rules for naming compounds). IUPAC work includes naming new elements and standardising methods of measuring things such as atomic weights. IUPAC encourages free sharing of scientific information.

Groups

Elements in the periodic table are arranged into vertical columns called groups. The group number of main group elements can be used to determine the number of valence electrons in an atom of the element.

In groups 1 and 2, the number of valence electrons is equal to the group number. For example, magnesium is in group 2 and therefore has two valence electrons.

In groups 13–18, the number of valence electrons is equal to the group number minus 10. For example, oxygen is in group 16, so oxygen has six valence electrons (outermost-shell electrons). Similarly, neon is in group 18, so neon has eight valence electrons. Helium is an important exception. It is located in group 18 but only has two valence electrons. Helium is placed in group 18 because it is unreactive, like other group 18 elements. This information is summarised in Table 4.1.1. Note that the numbers of valence electrons in groups 3–12 elements do not follow these patterns due to energy overlap of the outer *s* and *d* subshells.

TABLE 4.1.1 The number of valence electrons in elements belonging to each group

Group	Number of valence electrons
1	1
2	2
13	3
14	4
15	5
16	6
17	7
18	8*

*Helium has two valence electrons.

The valence electrons of an atom are the electrons that are involved in chemical bonding and chemical reactions. As a consequence, the number of valence electrons determines many of the chemical properties that an element exhibits.

Table 4.1.2 shows the names of some groups in the periodic table.

TABLE 4.1.2 Names of different groups in the periodic table

Group	Name
1	alkali metals
2	alkaline earth metals
17	halogens
18	noble gases

Elements in the same group have the same number of valence electrons, so elements in the same group have similar properties. For example, group 1 elements are the **alkali metals** (with the exception of hydrogen). They are all relatively soft metals and are highly reactive with water and oxygen.

Metals

Consider the **electron configurations** of the atoms of the first three metals of this group in Table 4.1.3. The valence shell of each atom of each element in group 1 contains one electron in an *s* subshell. This similarity in the valence shell structure gives these elements similar chemical properties.

TABLE 4.1.3 Electron configurations of selected metals in group 1

	Full electron configuration	Condensed electron configuration
Li	$1s^2 2s^1$	$[He]2s^1$
Na	$1s^2 2s^2 2p^6 3s^1$	$[Ne]3s^1$
K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$[Ar]4s^1$

Halogens

Fluorine, chlorine, bromine and iodine are **halogens** (group 17). They are all coloured and highly reactive (Figure 4.1.2). Their electron configurations are listed in Table 4.1.4. Notice how all these elements have a highest-energy subshell electron configuration of s^2p^5.

FIGURE 4.1.2 Three examples of halogens. These conical flasks contain, from left to right, chlorine gas (Cl, pale green), bromine gas (Br, red-brown) and iodine gas (I, purple).

TABLE 4.1.4 Electron configurations of selected halogens in group 17

	Full electron configuration	Condensed electron configuration
F	$1s^2 2s^2 2p^5$	$[He]2s^2 2p^5$
Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	$[Ne]3s^2 3p^5$
Br	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$	$[Ar]3d^{10} 4s^2 4p^5$
I	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^5$	$[Kr]4d^{10} 5s^2 5p^5$

Noble gases

The **noble gases** (group 18) are a particularly interesting group. The noble gases have a very stable electron arrangement: helium has a full valence shell and the other members of this group have a stable **octet arrangement** (eight electrons in the valence shell). Chemical reactions involve the rearrangement of valence electrons to achieve a stable valence shell. Noble gases have a stable electron configuration, so they do not tend to lose or gain electrons. This means that the noble gases are unlikely to undergo chemical reactions and have low **reactivity**.

The arrangement of electrons in atoms is responsible for the **periodicity** (or periodic trends) of element properties.

Periods

The horizontal rows in the periodic table are called periods. Periods are numbered 1–7. Like the group number, the number of a period gives information about the electron configuration of an element. The period an element is located within is equal to the number of occupied electron shells in the element's atoms. For example, the valence shell electrons of magnesium and chlorine reside in the third shell, and both of these elements are in period 3:

Mg $1s^2 2s^2 2p^6 3s^2$

Cl $1s^2 2s^2 2p^6 3s^2 3p^5$

Similarly, the elements in period 5 all have valence shell electrons in the fifth shell.

Blocks

The periodic table has four main **blocks,** as can be seen in Figure 4.1.3. The elements in each block have the same type of subshell (*s*, *p*, *d* or *f*) as their highest energy subshell. For example, the highest energy subshell of an element in the *s* block is the *s* subshell.

The *s* block contains the elements in group 1 (alkali metals), group 2 (**alkaline earth metals**), hydrogen and helium. These elements have a half-filled or fully filled *s* subshell (i.e. s^1 or s^2) as the highest energy subshell configuration. Table 4.1.5 and Figure 4.1.3 show which groups of elements fall into the four different blocks.

TABLE 4.1.5 Elements in the different blocks of the periodic table

Block	Elements	Highest energy subshell configurations
s	groups 1 and 2 and helium	s^1 or s^2
p	groups 13–18 (except helium)	s^2p^1 to s^2p^6
d	groups 3–12	d^1s^2 to $d^{10}s^2$
f	lanthanoids and actinoids	4*f* subshell progressively being filled in the lanthanoids 5*f* subshell progressively being filled in the actinoids

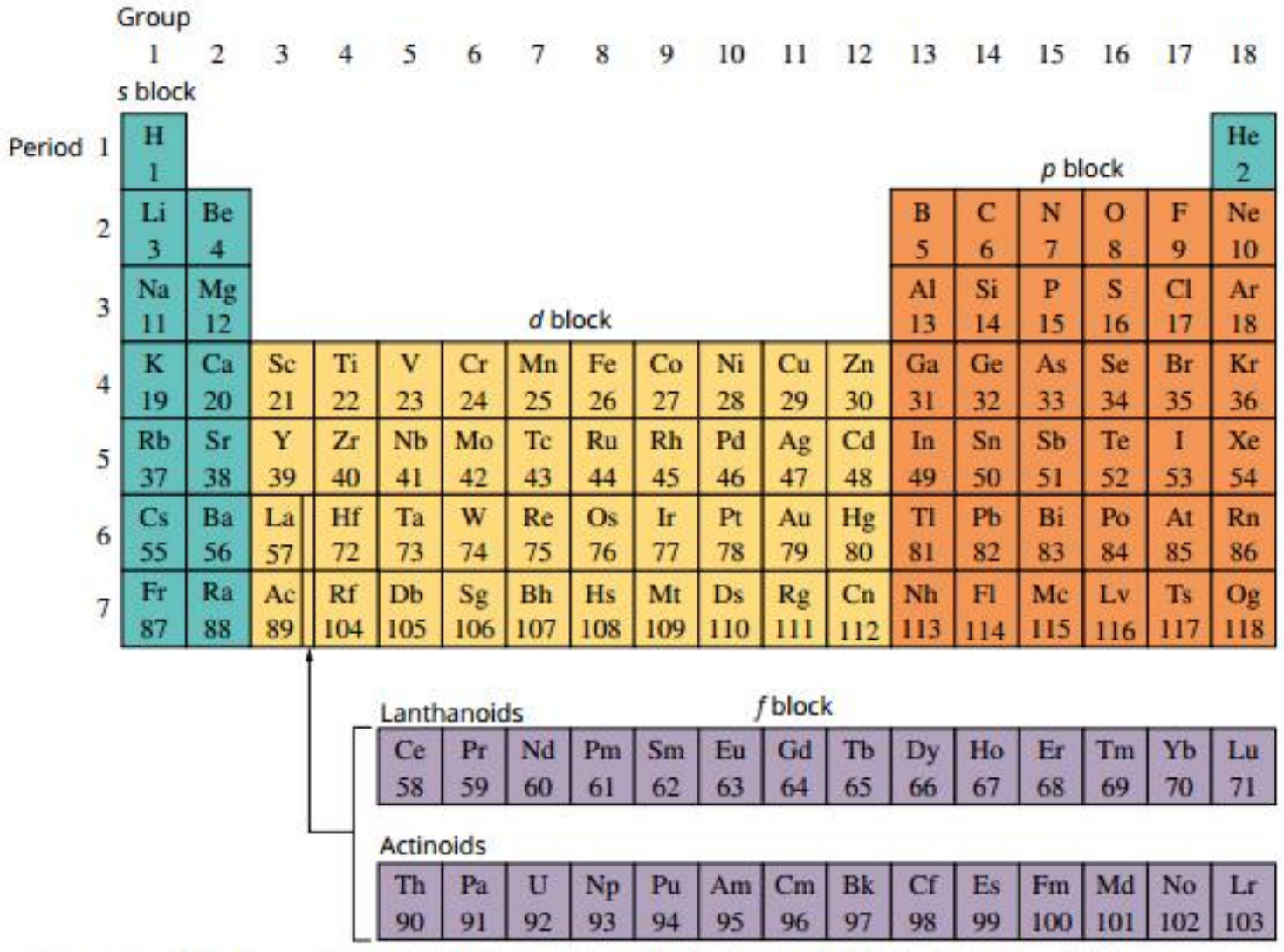


FIGURE 4.1.3 Colour is used to distinguish between the *s* (blue), *p* (orange), *d* (yellow) and *f* (purple) blocks of elements.

4.1 Review

SUMMARY

- The periodic table is a tool for organising elements according to their chemical and physical properties.
- The elements of the periodic table are arranged in order of increasing atomic number.
- Columns in the periodic table are known as groups and are numbered 1–18.
- The number of valence electrons in an atom of an element can be determined by the group in which it is located.
- The main group elements are in groups 1, 2 and 13–18 in the periodic table.
- Elements in between the main group elements (groups 3–12) are known as transition metals.
- Rows in the periodic table are known as periods and are numbered 1–7.
- The number of occupied electron shells of an atom of an element is equal to the number of the element's period.
- The periodic table has four main blocks of elements; the elements in each block have the same type of subshell (*s*, *p*, *d* or *f*) as their highest energy subshell.

KEY QUESTIONS

Describe

1 Define the terms 'period', 'group' and 'block'.

2 State the IUPAC name for the following groups with reference to the periodic table.

a group 1
b group 2
c group 17
d group 18

3 What is the number of valence electrons in the atoms of elements in each of these groups?

a group 1
b group 15
c group 17
d group 2

4 What are the highest energy subshells for *p* block elements?

5 What are the elements in the groups 3–12 known as?

Apply

6 Describe the key features of the periodic table.

7 Explain why noble gases have low reactivity.

Analyse

8 Determine the name and symbol of the following elements. In addition, identify the shell configuration and full electron configuration of each element.

a second element in group 14
b second element in period 2
c element that is in group 18 and period 3

9 Identify the period of the periodic table in which each of the following elements belongs. Use the periodic table in Figure 4.1.1 on page 50 as a reference.

a K
b F
c He
d H
e U
f P

10 Name three elements in the periodic table that have similar chemical properties to chlorine.

4.2 Periodic trends

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- recognise that the periodic trends are related to the electron configuration of the elements
- explain the concept of effective nuclear charge and its effect on the electrostatic attraction of the valence electrons
- define electronegativity and explain how it is affected by the effective nuclear charge across a period and down a group
- define atomic radius and explain how it is affected by the effective nuclear charge across a period and down a group
- define ionic radius and explain how it is affected by the effective nuclear charge across a period and down a group
- define the first ionisation energy and explain how it is affected by the effective nuclear charge across a period and down a group
- recognise the exceptions to the trend in the first ionisation energy and how the exceptions are related to the filling of the subshells.

The periodic table does not just provide information about an element's electron configuration. It can also be used as a tool for summarising the relative properties of elements and explaining the trends observed in those properties.

You have already seen in Module 4.1 that the group number of an element identifies how many valence electrons an atom of that element has. The period indicates how many electron shells are occupied in an atom of an element. Properties such as atomic radii, ionic radii, electronegativity and ionisation energy show common trends in the periodic table.

Periodic trends were observed by Dmitri Mendeleev and formed the basis of the table of the elements that he first published in 1869. Mendeleev described the way the properties of the elements vary as the periodic law. The modern form of the periodic law states that 'when the elements are arranged in order of increasing atomic number, elements with similar chemical and physical properties occur at periodic intervals'.

ELECTRON CONFIGURATION

To understand the reason for the periodicity of element properties, look at a group of elements that Mendeleev recognised as being similar. One such group is the alkali metals (group 1). The elements in this group (such as lithium, sodium, potassium, rubidium and caesium) are all relatively soft metals and are highly reactive with water and oxygen. Their electron configurations are shown in Table 4.2.1. These elements have similar valence shell electron configurations—all have one electron in an *s* subshell. Another group is the halogens (group 17). These elements (which include fluorine, chlorine, bromine and iodine) are all highly reactive. Their electron configurations are shown in Table 4.2.2. They all have five electrons in a *p* subshell. The similarity in a group's arrangement of electrons gives elements similar properties and is responsible for the periodicity of element properties.

TABLE 4.2.1 Electron configurations (full and condensed) for some elements in group 1, the alkali metals

	Full electron configuration	Condensed electron configuration
Li	$1s^2 2s^1$	$[He]2s^1$
Na	$1s^2 2s^2 2p^6 3s^1$	$[Ne]3s^1$
K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$[Ar]4s^1$
Rb	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 5s^1$	$[Kr]5s^1$
Cs	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6 6s^1$	$[Xe]6s^1$

TABLE 4.2.2 Electron configurations (full and condensed) for some elements in group 17, the halogens

	Full electron configuration	Condensed electron configuration
F	$1s^2 2s^2 2p^5$	$[He]2s^2 2p^5$
Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	$[Ne]3s^2 3p^5$
Br	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^5$	$[Ar]3d^{10} 4s^2 4p^5$
I	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^5$	$[Kr]4d^{10} 5s^2 5p^5$

You can also see that the number of electron shells occupied by electrons increases moving down a group. The increase in occupied shells means that the valence electrons are in higher energy subshells and have a weaker attraction to the nucleus. The decrease in the attractive force between the valence electrons and the nucleus as you move down a group causes trends in properties to be observed within a group.

EFFECTIVE NUCLEAR CHARGE

The **effective nuclear charge** of an atom is a measure of the attractive force felt by the valence shell electrons towards the nucleus. Effective nuclear charge can be used to predict some properties of elements and explain trends observed in the periodic table.

Consider an atom of lithium, which has an atomic number of three. It has three protons in its nucleus, two electrons in the first shell and one electron in the second shell (Figure 4.2.1).

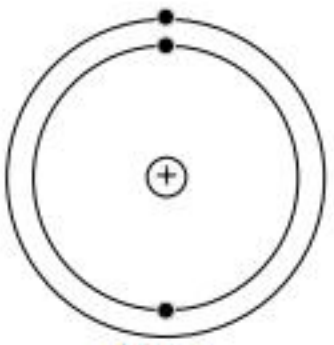


FIGURE 4.2.1 A lithium atom with one valence electron and two electrons in the inner shell. The atom has an effective nuclear charge of +1.

The valence shell electron is attracted to the three positive charges in the nucleus. This electron is also repelled by the two electrons in the inner shell. The electrons in the inner shell shield the valence shell electron from the attraction of the nucleus. The valence shell electron is effectively attracted to the nucleus as if there were a +1 nuclear charge. This atom is therefore said to have an effective nuclear charge of +1.

In atoms with two or more shells filled with electrons, the attraction between the nucleus and valence shell electrons is reduced by repulsion between the inner-shell electrons and the valence shell electrons. This is commonly known as the **shielding effect**.

> **In general: effective nuclear charge =**
> **number of protons in the nucleus – number of electrons in inner shells**

For example, an atom of chlorine (Figure 4.2.2) has 17 protons and seven valence shell electrons; the number of electrons in the inner shells is 10. The effective nuclear charge of a chlorine atom is 17 – 10 = +7.

Worked example 4.2.1

EFFECTIVE NUCLEAR CHARGE

Determine the effective nuclear charge of an atom of aluminium.	
Thinking	**Working**
Determine the number of electrons in an atom of the element, using the periodic table as a reference.	The atomic number of aluminium is 13. Therefore, an atom of aluminium has 13 protons and 13 electrons.
Use the number of electrons to determine the electron configuration.	With 13 electrons, the electron configuration is $1s^2 2s^2 2p^6 3s^2 3p^1$.
Determine the effective nuclear charge. Effective nuclear charge = number of protons − number of inner-shell electrons	The third shell is the valence shell in this atom. There are 10 inner-shell electrons, which in this atom are electrons in the first and second shells. Effective nuclear charge = 13 − 10 = +3

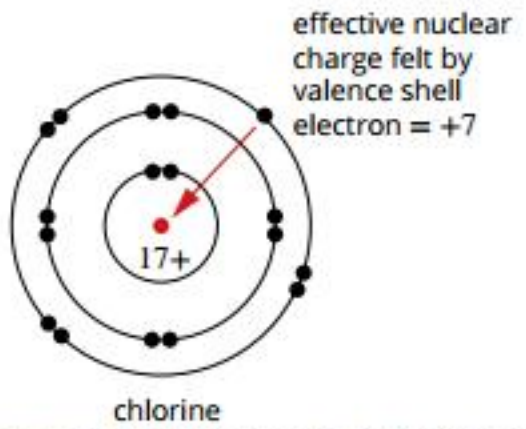


FIGURE 4.2.2 A Bohr diagram for the chlorine atom showing the valence shell electron shielded by 10 electrons in shells $n = 1$ and $n = 2$

➤ Try yourself 4.2.1

EFFECTIVE NUCLEAR CHARGE

Determine the effective nuclear charge of an atom of fluorine.

Consider the atoms of two different elements in group 1, lithium and sodium, as shown in Figure 4.2.3.

As for all group 1 elements, the valence electron of a lithium atom and a sodium atom experiences an effective nuclear charge of +1.

Moving down a group, you can see the following changes:

- The effective nuclear charge remains constant but the number of electron shells between the nucleus and valence electrons increases.
- The valence electrons are further from the nucleus. Consequently, they will be pulled less strongly towards the nucleus due to the reduced **electrostatic attraction** and increased repulsion from the inner-shell electrons (greater shielding effect).

Now consider sodium and chlorine. They are both in period 3 in the periodic table (Figure 4.2.4).

The effective nuclear charge experienced by the valence shell electrons in atoms of elements increases from left to right across a period, as you have seen for sodium and chlorine.

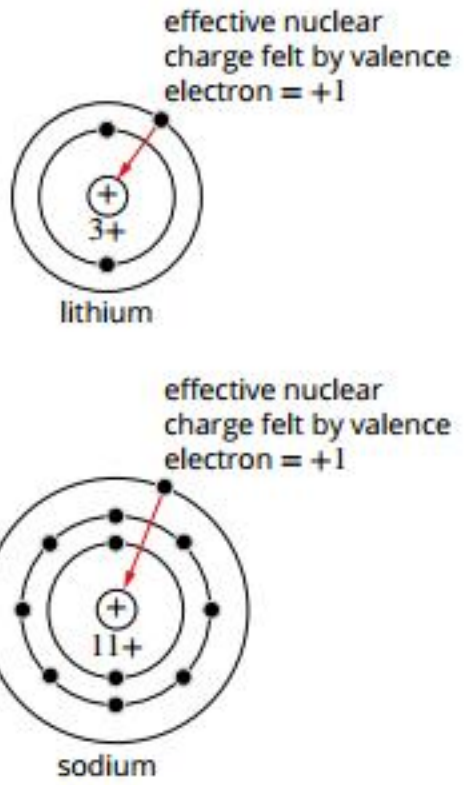


FIGURE 4.2.3 Lithium and sodium atoms both have an effective nuclear charge of +1.

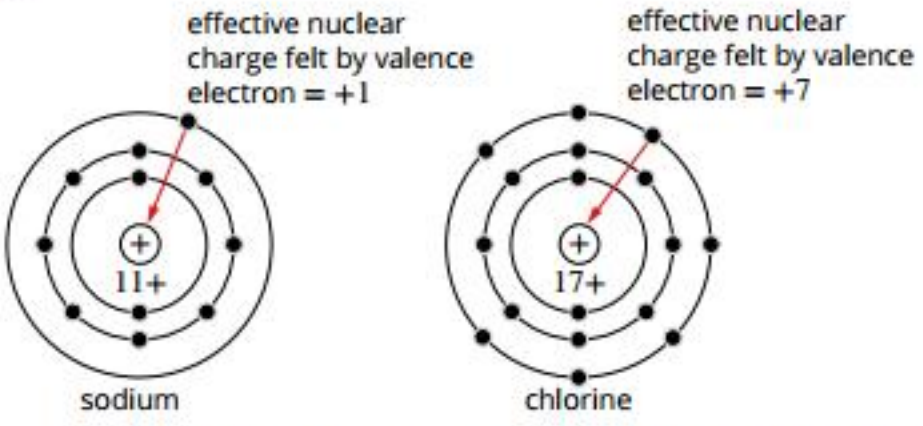


FIGURE 4.2.4 The effective nuclear charges of two period 3 elements, sodium and chlorine, are +1 and +7, respectively.

The effective nuclear charge of an atom of a main group element is equal to the number of valence electrons in the atom, as summarised in Table 4.2.3.

TABLE 4.2.3 Effective nuclear charges of main group elements

Group	Effective nuclear charge
1	+1
2	+2
13	+3
14	+4
15	+5
16	+6
17	+7
18*	+8

*Helium has an effective nuclear charge of +2.

Table 4.2.4 summarises how the attraction between the nucleus and valence electrons changes in the periodic table.

TABLE 4.2.4 The changes in attraction between the nucleus and valence electrons within groups and periods of the periodic table

	Trend in effective nuclear charge	Trend in attraction between the nucleus and valence electrons	Explanation for the trend in attraction between the nucleus and valence electrons
down a group	remains constant	decreases	Effective nuclear charge stays constant down a group, but the valence electrons are held less strongly as they are further from the nucleus, as there are more shells, and there is an increased shielding effect from the greater number of inner electron shells.
left to right across a period	increases	increases	The valence electrons are more attracted to the nucleus as the effective nuclear charge increases.

ELECTRONEGATIVITY

Electronegativity is the ability of an atom to attract valence electrons towards itself in a chemical bond. The main properties of an atom that determine its electronegativity are its atomic number and the size of the valence shell—which are both reflected in the effective nuclear charge. Therefore, in general, the greater the effective nuclear charge of an atom, the greater the electronegativity. Figure 4.2.5 shows the electronegativity of many of the main group elements. Although the concept of electronegativity is over 200 years old, nobody had been able to quantify it until Linus Pauling did so in 1932. Through a series of experimental observations and theoretical calculations, Pauling quantified electronegativity values and scaled them relative to a maximum value of 4.0 for fluorine. Figure 4.2.5 shows the values that Pauling found.

Electronegativity increases across a period →

Electronegativity decreases down a group ↓

1	2	13	14	15	16	17
Li	Be	B	C	N	O	F
1.0	1.6	2.0	2.6	3.0	3.4	4.0
Na	Mg	Al	Si	P	S	Cl
0.9	1.3	1.6	1.9	2.2	2.6	3.2
K	Ca	Ga	Ge	As	Se	Br
0.8	1.0	1.8	2.0	2.2	2.6	3.0
Rb	Sr	In	Sn	Sb	Te	I
0.8	1.0	1.8	2.0	2.0	2.1	2.7
Cs	Ba	Tl	Pb	Bi	Po	At
0.8	0.9	1.8	1.8	2.0	2.0	2.2
Fr	Ra					
0.7	0.9					

FIGURE 4.2.5 The electronegativity of elements generally decreases down a group and increases across a period, from left to right.

The trends observed in the electronegativity of the elements are summarised in Table 4.2.5.

TABLE 4.2.5 Trends in electronegativity in groups and periods of the periodic table

	Trend in electronegativity	Explanation
down a group	decreases	The effective nuclear charge stays constant and the number of shells increases down a group. Therefore, valence electrons are less strongly attracted to the nucleus as they are further from the nucleus. As a result, electronegativity decreases.
left to right across a period	increases	The number of occupied shells in the atoms remains constant, but the effective nuclear charge increases across a period. Therefore, the valence electrons become more strongly attracted to the nucleus. As a result, electronegativity increases.

ATOMIC RADIUS

Atomic radius is a measurement used to quantify the size of atoms. It can be regarded as the distance from the nucleus to the valence shell electrons. It is usually measured by halving the distance between the nuclei of two atoms of the same element that are bonded together. Figure 4.2.6 depicts the atomic radii of many of the main group elements. For example, in a hydrogen molecule (H_2), the two nuclei are 74 picometres (pm) apart. The radius of each hydrogen atom is assumed to be half of that distance, i.e. 37 pm.

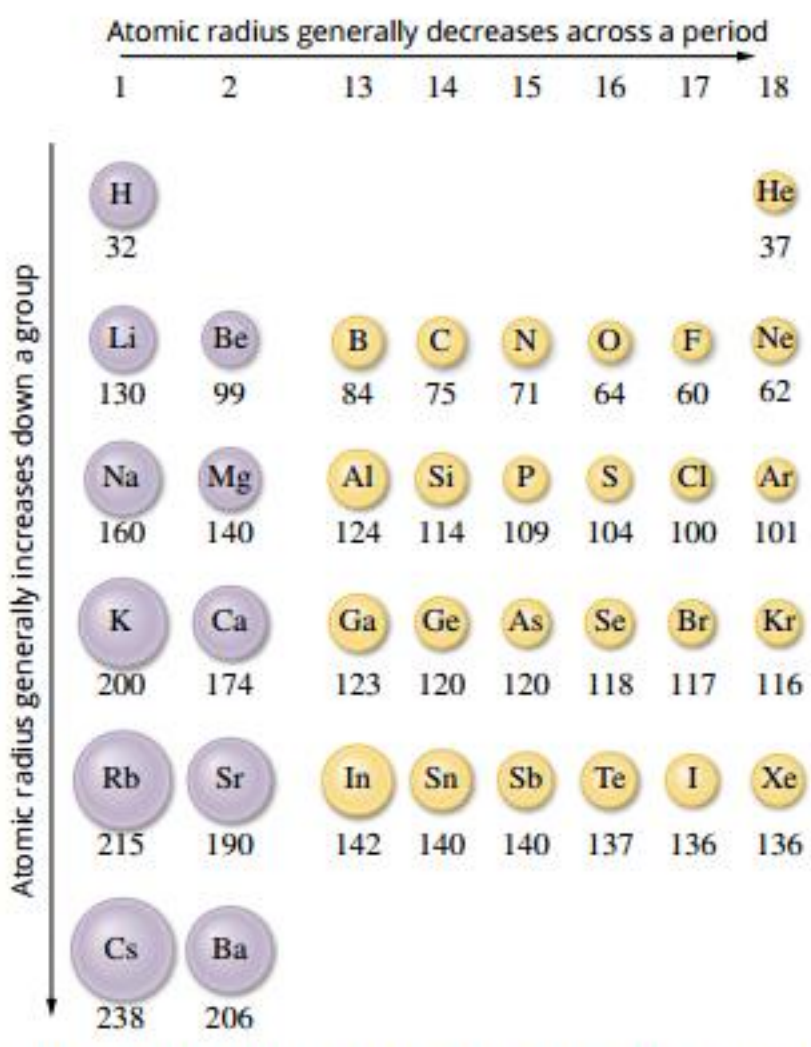


FIGURE 4.2.6 The relative sizes of atoms of selected main group elements. The atomic radii are given in picometres (pm). A picometre is 10^{-12} m.

Table 4.2.6 explains the trends in atomic radii in the periodic table.

TABLE 4.2.6 Trends in atomic radii in the periodic table

	Trend in atomic radii	Explanation
down a group	increases	Effective nuclear charge stays constant and the number of shells increases as you move down a group. As a result, atomic radii increase.
left to right across a period	decreases	As you move across a period, the number of occupied shells in the atoms remains constant, but the effective nuclear charge increases. The valence electrons become more strongly attracted to the nucleus, so atomic radii decrease across a period.

IONIC RADIUS

An ion is any atom of an element with a different number of protons than electrons. If an atom loses electrons, it becomes positively charged as there are now more protons than electrons. A positively charged ion is called a **cation**. If an atom gains electrons, it becomes negatively charged and is called an **anion**. You will learn more about ions in Chapter 7.

Atomic theory proposes that ions gain additional stability when they attain the electron configuration of a noble gas (group 18). Metallic elements tend to lose one or more electrons to form positive ions (cations), whereas non-metallic elements tend to gain electrons to form negative ions (anions). The **ionic radius** is defined as the radius of an atom's ion.

Similarly to the atomic radii, it is impossible to precisely determine the ionic radius. While it is possible to make a fairly reasonable assumption that the atomic radius is half the distance between atoms, this is not possible for ions.

Due to the large uncertainties in the actual dimensions, to compare ionic radii, it is necessary to use data from the same source. Despite the uncertainties, trends exist across a period and down a group.

Another trend in ionic radii is that cations are smaller than the parent atom from which they derived, and anions are larger than their parent atom. Consider a sodium atom, which has an atomic number of 11. It has a completely filled second shell and a single electron in the third shell. When it forms a cation, it loses the electron from the third shell to attain the electron configuration of neon. The effective nuclear charge increases due to the loss of the valence electron reducing the shielding effect. Also, there is a decrease in the repulsion between the electrons as there are fewer electrons in the valence shell. The combination of these two reasons explains why the cation has a much smaller radius than the sodium atom (102 pm compared to 160 pm) (Table 4.2.7).

TABLE 4.2.7 Electron configurations of the sodium atom and sodium cation

	Full electron configuration
Na	$1s^2 2s^2 2p^6 3s^1$
Na^+	$1s^2 2s^2 2p^6$

Moving across the period from sodium to magnesium, the effective nuclear charge increases. When magnesium forms an ion, it will generally lose both electrons from the third shell and attain the electron configuration of neon (Table 4.2.8).

TABLE 4.2.8 Electron configurations of the magnesium atom and magnesium ion

	Full electron configuration
Mg	$1s^2 2s^2 2p^6 3s^2$
Mg^{2+}	$1s^2 2s^2 2p^6$

The effective nuclear charge of a Mg^{2+} ion is higher than the effective nuclear charge of a Na^+ ion; therefore, the attraction between the nucleus and valence electrons increases from sodium to magnesium ions. Since the electron configurations of the ions formed are the same (**isoelectronic**) but the effective nuclear charge has increased, the size of the cations decreases, as shown in Table 4.2.9.

TABLE 4.2.9 Comparison of the effective nuclear charge and electron configuration of the cations in period 3

	Effective nuclear charge	Electron configuration of the stable cation	Ionic radius (pm)
Na^+	1	$1s^2 2s^2 2p^6$	102 pm
Mg^{2+}	2	$1s^2 2s^2 2p^6$	72 pm
Al^{3+}	3	$1s^2 2s^2 2p^6$	54 pm

Consider an atom of chlorine, which has an atomic number of 17 and five electrons in the third shell. When it forms an anion, it gains an electron to fill the third shell, attaining the electron configuration of argon (Table 4.2.10).

TABLE 4.2.10 Electron configurations of the chlorine atom and chlorine ion

	Full electron configuration	Ionic radius (pm)
Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	100 pm
Cl^-	$1s^2 2s^2 2p^6 3s^2 3p^6$	181 pm

The chloride ion has a greater number of valence electrons than the chlorine atom. This results in an increase in electron-electron repulsion in the electron cloud between the inner shells and valence shells and a decrease in effective nuclear charge. This, in turn, increases its size, and therefore increases the size of the overall ion, relative to the parent atom. The result is an ionic radius of 181 pm for the chloride ion, compared to 100 pm for the chlorine atom.

While the effective nuclear charge of the element increases as you cross the period from left to right, from sulfur to chlorine, the electron configuration of the anions formed is isoelectronic with the argon atom. In an identical way to the ionic radii of the cations, the valence electrons are more attracted to the nucleus as the effective nuclear charge increases. This means the ionic radius of the chloride ion is smaller than the ionic radius of the sulfide ions (181 pm compared to 184 pm).

Since the anions of period 3 gain electrons to complete the third shell (as opposed to the cations that lose their electrons from the third shell), the cations are much smaller than the anions formed by elements in the same period.

The trend down a group is similar to the trend in atomic radii. As the number of occupied electron shells increases, the valence electrons are further from the nucleus. This means that the ionic radius increases down the group. Table 4.2.11 explains the trends in ionic radii in the periodic table.

Atoms and ions of different elements that have the same electron configuration are said to be isoelectronic.

For instance, Mg^{2+} and Na^+ are isoelectronic.

TABLE 4.2.11 Trends in ionic radii in the periodic table

	Trend in ionic radii	Explanation
down a group	increases	Effective nuclear charge stays constant and the number of shells increases as you move down a group. As a result, ionic radii increase.
left to right across a period	decreases for species of the same charge	As you move across a period, the number of occupied shells in the ions remains constant for the species of the same charge, but the effective nuclear charge increases. The valence electrons become more strongly attracted to the nucleus, so ionic radii decrease across a period for the species of the same charge. Anions are larger than cations in the same period.

Figure 4.2.7 depicts the ionic radii of ions of many of the main group elements.

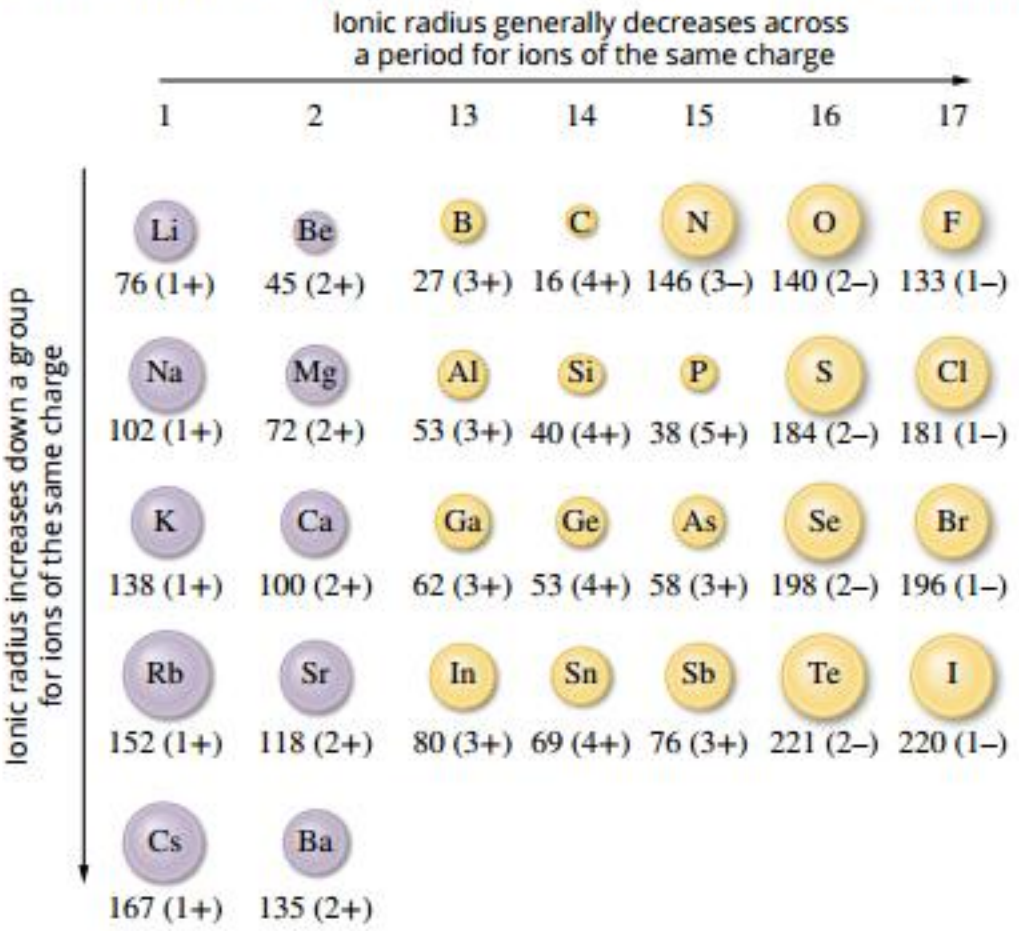


FIGURE 4.2.7 The relative sizes of common ions of selected main group elements. The ionic radii are given in picometres (pm). A picometre is 10^{-12} m. Where two ions are formed, the greater ionic radius of the more common ion is shown.

FIRST IONISATION ENERGY

When an element is heated, its electrons can move to higher energy shells. If an atom is given sufficient energy, an electron can be completely removed from the atom. If this occurs, the atom will now have one less electron than the number of protons in the nucleus, and becomes a cation as shown in the equation (where M is a generic element):

$$M(g) + \text{energy} \rightarrow M^+(g) + e^-$$

The process of removing an electron from an atom and forming an ion is called **ionisation**. The valence electrons are removed first because they are the furthest electrons from the nucleus and the least strongly held.

The energy required to remove one electron from an atom of an element in the gas phase is called the **first ionisation energy**. For example, the ionisation energy of sodium is 496 kJ per mole of sodium atoms.

Figure 4.2.8 shows the first ionisation energies of the first 86 elements.

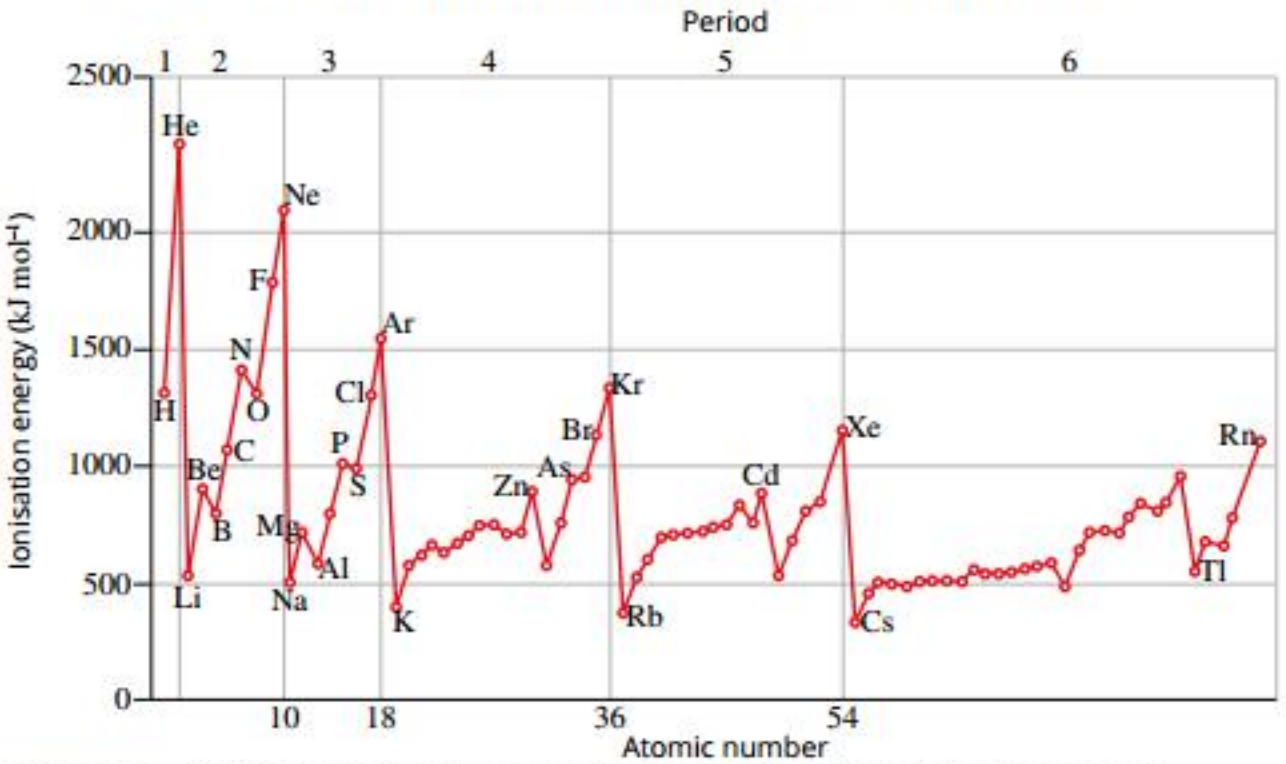


FIGURE 4.2.8 The first ionisation energy generally increases from left to right across a period.

The magnitude of the first ionisation energy reflects how strongly the valence electrons are attracted to the nucleus of the atoms. The more strongly the valence electrons are attracted to the nucleus, the more energy is required to remove them from the atom and the higher the first ionisation energy. Table 4.2.12 explains the typical trends in ionisation energy in the periodic table.

TABLE 4.2.12 Trends in ionisation properties in groups and periods of the periodic table

	Trend in ionisation energy	Explanation
down a group	decreases	Effective nuclear charge stays constant and the number of shells increases down a group. Therefore, the valence electrons are less attracted to the nucleus as they are further from the nucleus. As a result, the energy required to overcome the attraction between the nucleus and the valence electron is less, and the first ionisation energy decreases down a group.
left to right across a period	increases	Effective nuclear charge increases and the number of occupied shells remains constant across a period. As a result, the valence electrons become more strongly attracted to the nucleus, and more energy is required to remove an electron. Therefore, the first ionisation energy increases across a period.

The *s* and *p* block elements of the periodic table follow these patterns. As the effective nuclear charge increases across a period, so too does the ionisation energy. Down a group, the effective nuclear charge stays the same, but the increased atomic radius and greater shielding effect from the inner electron shells means that the valence electrons in elements lower in a group have a smaller electrostatic attraction to the nucleus. Therefore, they can be removed more easily, meaning the ionisation energy decreases.

Exceptions to the rule

As you have seen, across a period, the first ionisation energy increases due to the increase in the effective nuclear charge; however, there are two exceptions to this trend in period 2. There is a decrease from 900 to 801 kJ mol^{-1} going from beryllium (Be) to boron (B) and a decrease from 1402 to 1314 kJ mol^{-1} going from nitrogen (N) to oxygen (O). To understand these exceptions better, you first need to determine the electron configuration of the elements involved. Table 4.2.13 shows the electron configurations of the beryllium and boron atoms.

TABLE 4.2.13 Electron configurations of the beryllium and boron atoms

	Full electron configuration
Be	$1s^2 2s^2$
B	$1s^2 2s^2 2p^1$

The electron that is removed from beryllium comes from a full *s* subshell, whereas the electron that is removed from boron comes from a *p* subshell. In Module 3.3, you saw that the *p* subshell is higher in energy than the *s* subshell within a given shell. In addition, the filled 2*s* subshell shields the $2p^1$ electron in the *p* subshell, so the electrostatic attraction of the nucleus is reduced. These two factors mean that less energy is required to remove the electron from the 2*p* subshell, and so the first ionisation energy of B is lower than that of Be, even though the atom has a greater effective nuclear charge.

You have also seen in Module 3.3 that as you cross a period in the periodic table, the added electrons enter unfilled orbitals until all the orbitals in the same subshell contain one electron (Hund's rule). In nitrogen, the three electrons are in the three different *p* orbitals; however, when an atom of oxygen is ionised the electron is removed from a filled *p* orbital. The electron configurations of the nitrogen and oxygen atoms are shown in Table 4.2.14. Since like charges repel, when two electrons are in close proximity to one another, the electrons are destabilised. Even though the electron that is removed from oxygen is higher in energy than the electron in nitrogen, the first ionisation energy of oxygen is lower than the first ionisation energy of nitrogen.

TABLE 4.2.14 Electron configurations of the nitrogen and oxygen atoms

	Full electron configuration
N	$1s^2 2s^2 2p^3$
O	$1s^2 2s^2 2p^4$

4.2 Review

SUMMARY

- The effective nuclear charge of an atom is a measure of the attractive force felt by the valence electrons towards the nucleus.
- The effective nuclear charge is calculated by subtracting the total number of inner-shell electrons from the number of protons in the nucleus.
- Electronegativity is the ability of an atom to attract valence electrons towards itself in a chemical bond. In general, the greater the effective nuclear charge of an atom, the greater the electronegativity.
- Atomic radius is a measurement used to quantify the size of atoms. It can be regarded as the distance from the nucleus to the valence shell electrons.
- Ionic radius is a measurement used to quantify the size of ions. It is measured either experimentally or calculated theoretically as the distance between the nucleus and outermost electrons.
- The first ionisation energy is the energy required to remove one electron from an atom of an element in the gas phase and is represented by the equation

$$M(g) + \text{energy} \rightarrow M^+(g) + e^-$$

- Table 4.2.15 summarises how properties of elements have specific trends within the groups and periods of the periodic table.

TABLE 4.2.15 Summary of changes in properties of elements in the periodic table

Property	Down a group	Left to right across a period
effective nuclear charge	no change	increases
atomic radius	increases	decreases
ionic radius	increases	decreases for species of the same charge; larger for anions than cations in the same period
electronegativity	decreases	increases
first ionisation energy	decreases	increases

KEY QUESTIONS

Describe

1 Define the term 'effective nuclear charge' of an atom.

2 Define the first ionisation energy of an atom.

3 Which *p* block element has the smallest atomic radius? Refer to Figure 4.2.6 on page 59.

4 Which element has the highest first ionisation energy? Refer to Figure 4.2.8 on page 63.

Apply

5 Explain the term 'shielding effect'.

6 Explain the relationship between electronegativity and effective nuclear charge.

7 Figure 4.2.5 on page 58 gives electronegativity values for the elements in groups 1, 2 and 13–17.

a Determine the element that has the:

i highest electronegativity

ii lowest electronegativity.

b Identify the group which has the following changes:

i greatest change in electronegativity as you go down the group

ii smallest change in electronegativity as you go down the group.

c Explain why the elements of group 18 are usually not shown in tables of electronegativity values.

8 Explain why the size of the Al^{3+} cation is different from the size of the parent atom from which it was formed.

9 Which group has an effective nuclear charge of +6?

Analyse

10 Calculate the effective nuclear charge on atoms of:

a carbon

b sodium

c fluorine

d helium.

11 Compare and contrast the trends in atomic and ionic radii in the periodic table using specific examples.

12 Organise the following elements in order of increasing first ionisation energies, using the periodic table on page 50 (Figure 4.1.1): Na, He, Al, K, Cl and P.

13 Predict whether Mg^{2+} is larger than F^- using the periodic table on page 50 (Figure 4.1.1). Explain your choice based on the structure of the two ions.

14 Explain why the number of subatomic particles in an atom increases across a period, but the size of the atom decreases.

15 Referring to Figure 4.2.8, which of the first 36 elements have a first ionisation energy between 900 and 1100 kJ mol^{-1}?

4.3 Relating periodic trends and atomic properties

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- use the periodic table to determine which elements are metals, metalloids and non-metals
- compare and explain differences in the reactivity of the alkali metals as you go down group 1
- compare and explain differences in the reactivity of the halogens as you go down group 17
- explain how the differences in the reactivity of the alkali metals are related to the trends in ionisation energy of the elements
- explain how the differences in the reactivity of the halogens are related to the trends in electron affinities of the elements
- recognise how the nature of period 3 oxides changes from basic through amphoteric to acidic.

You have learnt that the effective nuclear charge and the number of electron shells in an atom of an element can be used to predict some properties of elements. Remember that the effective nuclear charge of an atom is the attractive force felt by the valence electrons towards the nucleus. Effective nuclear charge increases as you move across a period. As you move down a group, the effective nuclear charge stays constant, but the atomic radius increases due to the additional electron shell in each period. The changes in effective nuclear charge and atomic radii account for periodic trends in ionisation energy, reactivity and metallic character.

METALLIC CHARACTER

Metallic character of an element is defined as the ease with which its atoms lose electrons. Therefore, metallic character is related to the ionisation energy of the element. Metals conduct electricity and are usually solids at room temperature. Conversely, non-metallic elements usually do not conduct electricity, and many are gases at room temperature.

The differences between the properties of metals and non-metals are related to the number of electrons in the valence shell of their atoms. In general, elements with atoms containing one, two or three valence electrons tend to behave as metals, whereas those with four or more valence electrons behave as non-metals. You will study this in more detail in Chapters 6–8. For now, however, you can note that the metallic character of elements generally increases as you go down a group and decreases as you go from left to right across a period.

Metalloids

Many periodic tables have a solid jagged line with metals located to the left side and non-metals to the right (Figures 4.1.1 and 4.3.1). Elements known as the **metalloids** are located adjacent to this line, separating the metals and non-metals. The metalloids exhibit both metallic and non-metallic properties. Silicon is one of the most abundant metalloids. It is a brittle solid, which is a common property of non-metals. However, it is also a semiconductor, meaning it conducts electricity (a property of metals), making it useful in many electronic devices such as computers and calculators.

REACTIVITY

The reactivity of an element is an indication of how easily an atom of that element undergoes chemical change by losing, gaining or sharing electrons.

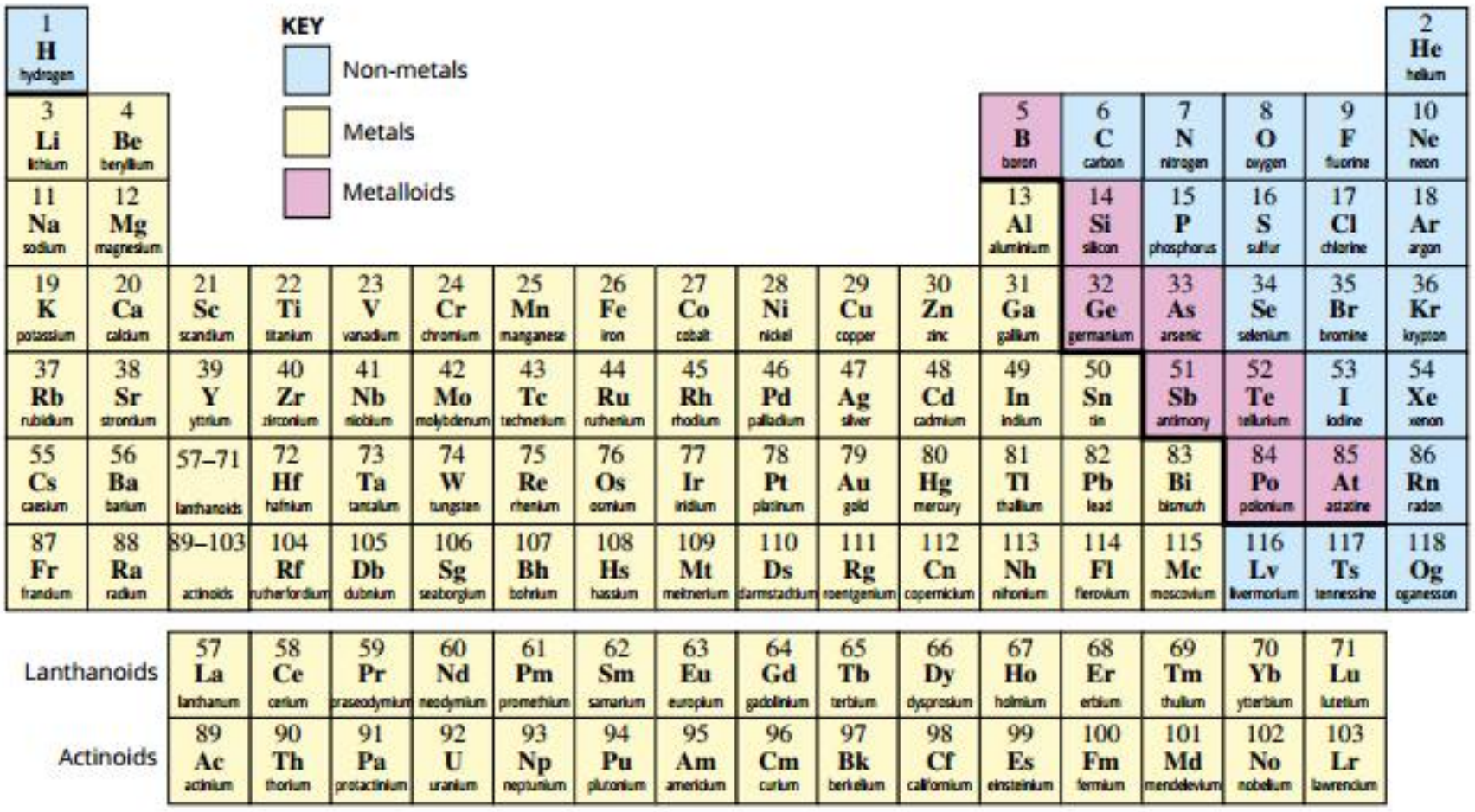


FIGURE 4.3.1 A periodic table showing the metals, metalloids and non-metals. The jagged black line separates the metals (left) from the non-metals (right). Note: hydrogen is a non-metal.

Reactivity of metals

When metals react, they tend to lose electrons. Therefore, the reactivity of metals is a measure of how easily an atom of a metallic element can lose electrons. The weaker the attraction of the valence electrons to the nucleus, the more easily the electrons can be lost.

Moving down a group, the electrostatic attraction between the nucleus and valence electrons decreases due to the increasing number of electron shells in the atoms. This means that reactivity of metals increases down a group. The rate at which metals react with water indicates their relative reactivity.

From left to right across the periodic table, the effective nuclear charge of the atoms increases, and it becomes more difficult for the element to lose electrons. Within the metals, this means there is a decrease in reactivity. This agrees with the observations from Table 4.3.1, which describes the reaction of some of the group 1 and 2 metals with water. Table 4.3.1 shows that the group 1 metals are more reactive than the group 2 metals. The table also shows that the reactivity with water increases from sodium through potassium to rubidium, that is, as the period increases from 3 to 5.

TABLE 4.3.1 Reaction of some group 1 and 2 metals with water. In each case, a reaction results in the formation of hydrogen gas.

Period	Group	Element	Reaction with water
3	1	sodium	vigorous, producing enough energy to melt the sodium, which fizzes and skates on the water surface
4	1	potassium	violent, making crackling sounds as the heat evolved ignites the hydrogen produced by the reaction
5	1	rubidium	violent explosion
3	2	magnesium	no reaction at room temperature, but will react with steam
4	2	calcium	slow reaction at room temperature

In summary, the reactivity of metals:

- increases down a group as it is easier for a metal with a greater number of shells to lose electrons
- decreases across a period as the increasing effective nuclear charge makes it more difficult for a metal to lose electrons.

Reactivity of non-metals

Atoms of non-metallic elements undergo chemical reactions to gain or share electrons to form a stable electron configuration of eight electrons in the valence shell (octet arrangement). The more easily a non-metal can gain or share electrons to achieve a stable electron configuration, the more reactive that non-metal is. Non-metallic elements with higher electronegativity values will have a greater attractive force for valence electrons of other atoms, and thus be more reactive.

Therefore, the reactivity trends of non-metals mirror the electronegativity trends:

- Chemical reactivity decreases down a group as it is harder for a non-metal atom to attract electrons (either by gaining or sharing) into the larger valence shell when a greater number of shells are occupied.
- Chemical reactivity increases across a period as the increasing effective nuclear charge makes it easier for a non-metallic atom to attract valence electrons from other atoms (either by gaining or sharing).

Change in the nature of the oxides across a period

An **ionic bond** is formed between two atoms when there is a large difference in electronegativity (greater than 1.8) between two elements. Since oxygen is highly electronegative, it forms ionic bonds with all metals.

Therefore, across a period (from left to right), the oxides go from ionic to covalent. This trend is most obvious for the elements in periods 2 and 3. Table 4.3.2 shows the trend in period 3.

TABLE 4.3.2 Relationship between the electronegativity difference, bonding and acidic nature of the oxide of elements in period 3

Element	Electronegativity	Electronegativity difference[1]	Bonding	Acidic nature of the oxide
sodium	0.9	2.5	ionic	strong base
magnesium	1.3	2.1	ionic	weak base
aluminium	1.6	1.8	ionic	amphoteric
silicon	1.9	1.5	covalent	weak acid
phosphorus	2.6	1.2	covalent	strong acid
sulfur	2.6	0.8	covalent	strong acid
chlorine	3.2	0.2	covalent	strong acid

[1]Electronegativity of oxygen is 3.4.

The acidic nature of the oxides changes across the period and this can be observed through the reaction of the oxide with water. Table 4.3.3 describes the reaction of some of the oxides of period 3 elements with water to highlight the acidic nature of the oxide.

TABLE 4.3.3 Reaction of some of the period 3 oxides with water

Group	Element	Reaction of the oxide with water
1	sodium	highly soluble; reacts exothermically (releases heat) to form a highly basic solution of sodium hydroxide
2	magnesium	slightly soluble; reacts to form a weakly basic solution of magnesium hydroxide
3	aluminium	insoluble in water; reacts with both acids and bases, so is termed **amphoteric**
4	silicon	completely insoluble in water; reacts with very strong bases, so it is a weakly acidic oxide
5	phosphorus	the two oxides of phosphorus, P_2O_3 and P_2O_5, react with water to form strongly acidic solutions
6	sulfur	the two oxides of sulfur, SO_2 and SO_3, react with water to form strong acids
7	chlorine	reacts to form a very strong acid

4.3 Review

SUMMARY

- In chemical reactions, metals tend to lose electrons and non-metals tend to gain or share electrons.
- From left to right across a period, the elements change from metals to metalloids to non-metals.
- Chemical reactivity is the ease with which an element undergoes a reaction.
- Chemical reactivity of metals increases down a group, but decreases across a period and is related to the trends in ionisation energy.
- Chemical reactivity of non-metals decreases down a group, but increases across a period and is related to the trends in electronegativity.
- The nature of the oxides changes from basic through amphoteric to acidic across period 3.
- Many trends in the physical and chemical properties of elements in the periodic table can be explained using two key ideas.
  - From left to right across a period, the effective nuclear charge of atoms increases, so that the attractive force felt between the valence electrons and the nucleus increases.
  - Down a group, the number of shells in an atom increases, so that the valence electrons are further from the nucleus and are held less strongly.

KEY QUESTIONS

Describe

1 Identify whether the following elements are metals, metalloids or non-metals using the periodic table on page 67.

a K
b N
c Ge
d Cu
e Sn
f I

2 What is an amphoteric substance?

3 What is a metalloid?

Apply

4 Determine whether the oxides of the following elements will be acidic, basic or amphoteric.

a C
b Li
c Ca
d Br

5 Explain the difference in reactivity with water between lithium and caesium.

6 An atom that is not helium has two electrons in its valence shell. Will this element be a metal, metalloid or non-metal?

Analyse

7 Arrange the following elements in order of increasing reactivity:
P, Cl, Ar, S.

8 Analyse the elements in period 2.
Describe the changes in the following properties across the period.

a the sizes of atoms
b metallic character
c electronegativity

9 Explain why the reactivity of beryllium is less than that of barium.

4.4 Introduction to bonding

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- recognise that bonding is caused by the electrostatic attraction between oppositely charged species
- recognise that the position of the elements in the periodic table determines the nature of the chemical bonds formed
- recognise that ionic bonds are formed between metal and non-metal atoms
- recognise that covalent bonds are formed between non-metal atoms
- recognise that metallic bonds are formed between metal atoms
- recognise that arrangement of electrons in atoms and stability of valence electron shells determine the ability of atoms to form chemical bonds.

When elements combine to form a compound, there are three major types of bonding that can result.

- **Covalent bonds** are the result of sharing of valence electrons between non-metallic atoms.
- **Metallic bonds** are the result of the electrostatic attraction of **delocalised** valence electrons shared across a lattice of metal cations.
- Ionic bonds are the result of the electrostatic attraction between positively charged ions (cations) and negatively charged ions (anions).

The ability of atoms to form chemical bonds, and the type of bonds they form, are related to both the number and configuration of valence electrons. Generally, noble gases do not form bonds because they have stable valence electron shells. These group 18 elements do not need to gain, lose or share electrons to form the stable octet of valence electrons (or for helium, a stable pair of valence electrons). Elements with a low number of valence electrons (1–3) generally form metallic or ionic bonds (by sharing electrons with other metal atoms or losing electrons to form a positively charged cation); whereas elements with a high number of valence electrons (4–7) generally form covalent or ionic bonds (by sharing electrons with other atoms or gaining electrons to form a negatively charged anion).

WHEN ATOMS COMBINE

In Module 4.3, you learnt that metals are found to the left of the solid 'staircase' line in the periodic table, with non-metals found to the right of the line (Figure 4.3.1 on page 67).

Covalent bonding happens when non-metals combine with other non-metals, resulting in the formation of groups of atoms known as molecules. While non-metals have the ability to remove electrons from metals, they cannot do this to other non-metals. Instead, they tend to share electrons in covalent bonds, resulting in the formation of molecules. Covalent bonds occur when two non-metal atoms share one or more pairs of valence electrons. This creates an electrostatic attraction between the two nuclei that holds the atoms together in a covalent bond (Figure 4.4.1). As hydrogen is a non-metal, when it is combined with another non-metal, it will also produce a covalent bond. Non-metals only share enough electrons to fill their valence shell or to achieve an octet of valence electrons. For example, nitrogen has five valence electrons, so must pair up three of its electrons with electrons from other non-metallic elements. Covalent bonding will be covered in greater depth in Chapter 8.

A covalent bond results from the sharing of electrons between two non-metallic atoms.

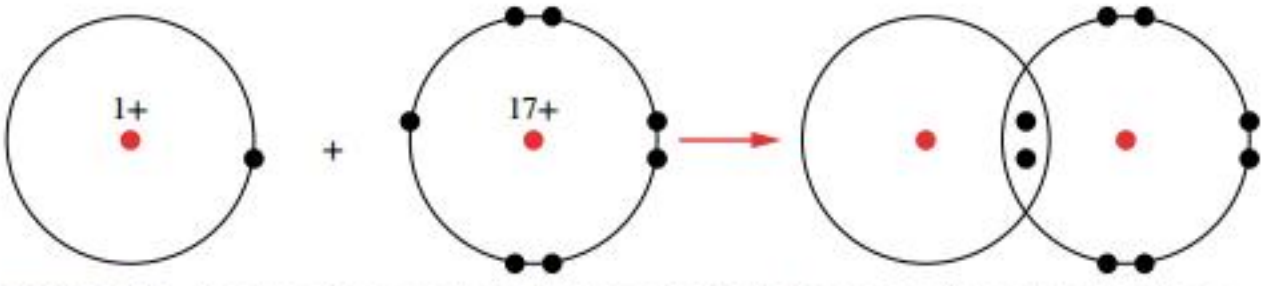


FIGURE 4.4.1 Hydrogen has one valence electron and chlorine has seven valence electrons. A pair of electrons is shared to fill the valence shells of both atoms, resulting in the formation of a molecule of HCl.

When metal atoms combine with each other, they form metallic bonds. Metal atoms have a weak hold on their valence electrons. This gives the valence electrons the freedom to be shared throughout the metal lattice of cations without being bound to any one nucleus. In this case, each metal atom donates its valence electrons to create a mobile 'sea' of electrons that are not localised on a particular atom (or nucleus), but are able to be shared across the metal lattice structure. The relatively free movement of electrons is the reason for the typical characteristics of metals such as conductivity, malleability and lustrousness, as shown in Figure 4.4.2. The attraction between the metal cations and the negatively charged electrons holds the metal lattice together. A pure metal is one in which only one type of metal atom is present; however, if more than one type of metal atom is present, then an alloy is formed. Metallic bonding will be covered in greater detail in Chapter 6.

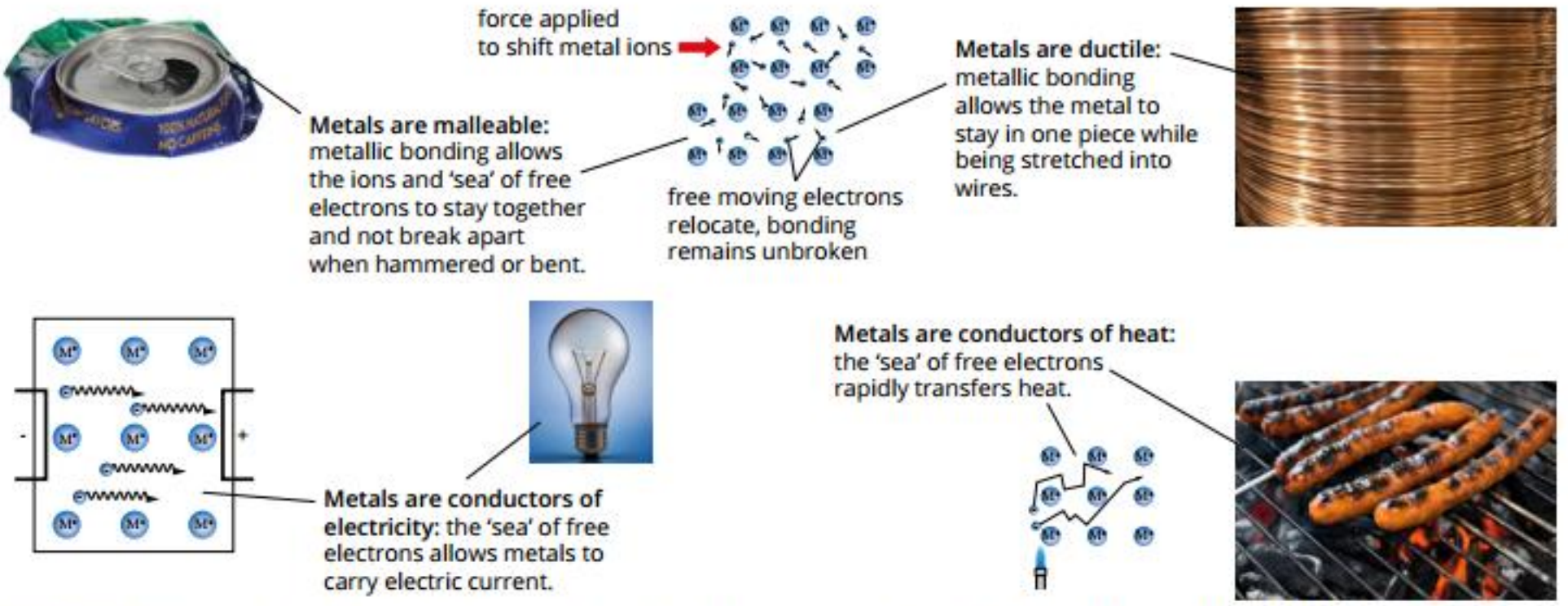

force applied
to shift metal ions
Metals are malleable: metallic bonding allows the ions and 'sea' of free electrons to stay together and not break apart when hammered or bent.
free moving electrons relocate, bonding remains unbroken
Metals are ductile: metallic bonding allows the metal to stay in one piece while being stretched into wires.
Metals are conductors of electricity: the 'sea' of free electrons allows metals to carry electric current.
Metals are conductors of heat: the 'sea' of free electrons rapidly transfers heat.

FIGURE 4.4.2 Each metal cation is attracted to a 'sea' of delocalised valence electrons released from all metal atoms within the lattice. This mutual attraction bonds the metal together.

A metallic bond is the attraction of the stationary metal cations to the surrounding delocalised electrons.

In Module 4.2, you learnt that metals have low ionisation energies, meaning that they lose electrons relatively easily to form positively charged cations. Non-metals have high ionisation energies, so have a tendency to gain electrons relatively easily (rather than losing them), forming negatively charged anions.

Therefore, when a metal and non-metal are combined, electron transfer from metal atoms to non-metal atoms is possible, forming positively charged cations and negatively charged anions. The electrostatic attraction between ions of opposite charge creates a three-dimensional structure called a lattice, where each ion is surrounded by ions of opposite charge. The process is shown in Figure 4.4.3.

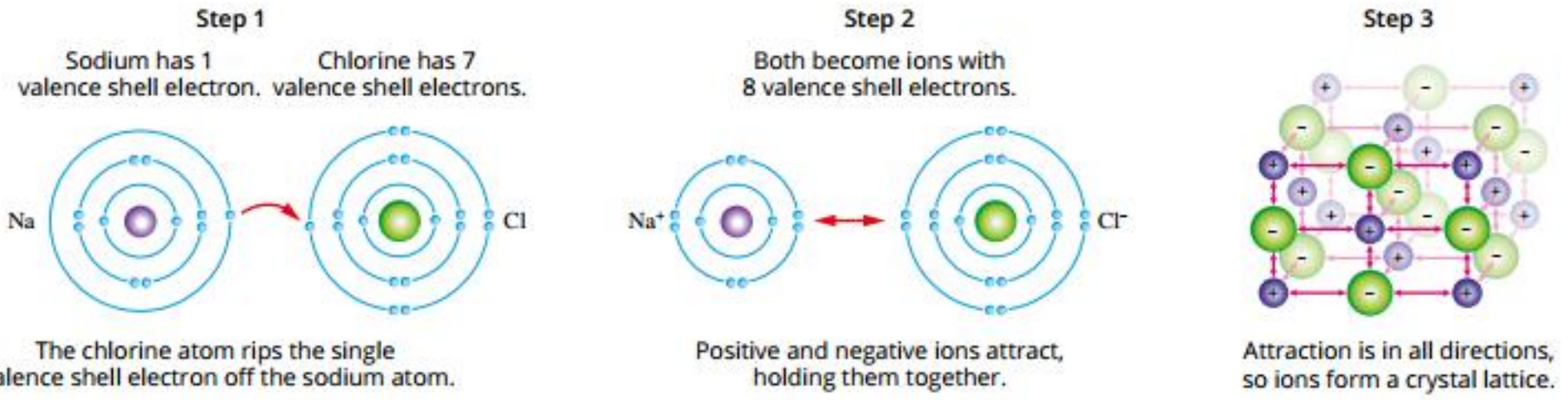

Step 1
Sodium has 1 valence shell electron.
Chlorine has 7 valence shell electrons.
Na
Cl
The chlorine atom rips the single valence shell electron off the sodium atom.
Step 2
Both become ions with 8 valence shell electrons.
Na+
Cl−
Positive and negative ions attract, holding them together.
Step 3
Attraction is in all directions, so ions form a crystal lattice.

FIGURE 4.4.3 Ionic bonding holds table salt (sodium chloride, NaCl) together.

Elements in the same group tend to lose or gain the same number of electrons when they react. This means they form ions of the same charge. For example, every element in group 1 forms an ion carrying a +1 charge when it bonds with a non-metal. Likewise, the elements of group 17 gain a single electron to get a −1 charge. The oppositely charged ions create an electrostatic attraction known as an ionic bond. Ionic bonding is covered in more detail in Chapter 7.

In summary, you can use the periodic table to determine whether the substances are composed of metals and/or non-metals, making it possible to predict the type of bonding present in the substance.

An ionic bond results from the electrostatic attraction between two oppositely charged ions.

Ionic bonding occurs between metal and non-metal atoms.
Covalent bonding occurs between non-metal atoms.
Metallic bonding occurs between metal atoms.

4.4 Review

SUMMARY

- Metals are on the left side of the periodic table.
- Non-metals are on the right side of the periodic table.
- Covalent bonds involve two non-metals.
- Ionic bonds involve a non-metal and a metal.
- Metallic bonds (including alloys) involve two metals.
- An ionic bond is formed through an electrostatic attraction between two oppositely charged ions.
- A covalent bond involves one or more pairs of electrons being shared between two atoms.
- Metals have a 'sea' of delocalised electrons shared across multiple metal atoms.

KEY QUESTIONS

Describe

1 What is a covalent bond?

2 Define 'delocalised electrons' in metallic bonding.

Apply

3 Would you find non-metals on the left- or right-hand side of the periodic table?

Analyse

4 Classify the bond between each of the following pairs of atoms as covalent, ionic or metallic using the periodic table (Figure 4.3.1 on page 67).

a sodium and chlorine atoms
b magnesium and aluminium atoms
c nitrogen and oxygen atoms
d aluminium and sulfur atoms
e hydrogen and lithium atoms
f fluorine and chlorine atoms
g two sulfur atoms

5 Predict the type of chemical bond that will form between:

a two copper atoms
b two chlorine atoms
c two sodium atoms
d two hydrogen atoms.

6 Explain why aluminium ions and calcium atoms cannot form an ionic bond between them.

Chapter review

04

KEY TERMS

alkali metal
alkaline earth metal
amphoteric
anion
atomic number
atomic radius
block (periodic table)
cation
covalent bond
delocalise
effective nuclear charge
electron configuration
electronegativity
electrostatic attraction
first ionisation energy
group (periodic table)
halogen
ionic bond
ionic radius
ionisation
isoelectronic
main group element
metallic bond
metallic character
metalloid
noble gas
octet arrangement
period (periodic table)
periodic table
periodic trend
periodicity
reactivity
shielding effect
transition metal
valence electron

KEY QUESTIONS

Describe

1 What is the symbol for the element iron?

2 What is the name of the element with the symbol K?

3 Define an ionic bond.

4 Which response best describes how the elements in the periodic table are arranged?
- **A** by the number of neutrons in their nucleus
- **B** by the number of protons in their nucleus
- **C** by increasing mass number
- **D** by increasing atomic mass

5 Identify the element whose properties are most similar to sodium.
- **A** magnesium
- **B** aluminium
- **C** potassium
- **D** hydrogen
- **E** silicon

6 Identify the response that correctly shows increasing radius of the following species.
- **A** Cl^-, Ca^{2+}, K^+
- **B** Ca^{2+}, K^+, Cl^-
- **C** Cl^-, K^+, Ca^{2+}
- **D** Ca^{2+}, Cl^-, K^+

7 Identify the most reactive non-metal from the following elements.
- **A** caesium
- **B** chlorine
- **C** fluorine
- **D** oxygen
- **E** sulfur

8 A 'sea of delocalised electrons' is a feature of which type of chemical bonding?
- **A** ionic
- **B** basic
- **C** covalent
- **D** metallic

9 Use the periodic table in Figure 4.1.3 on page 53 to determine the period and block of the following elements.
- **a** hydrogen
- **b** carbon
- **c** phosphorus
- **d** copper
- **e** uranium

10 What is the number of valence electrons in an atom of germanium?

11 Identify the effective nuclear charge of nitrogen.

12 Identify whether the following oxides are acidic, basic or amphoteric.
- **a** aluminium oxide
- **b** sodium oxide
- **c** sulfur dioxide

13 Select the appropriate word from the following options to complete the sentences below: increases, decreases.
- **a** The force of attraction between the nucleus and valence electrons _____ in a period from left to right.
- **b** Atomic radii of elements _____ in a period from left to right.
- **c** Atomic radii of elements _____ in a group from top to bottom.
- **d** Metallic character of elements _____ in a group from top to bottom.

Apply

14 Nitrogen is found in period 2 and group 15 of the periodic table.
- **a** Explain the difference between the terms 'period' and 'group'.
- **b** State the electron configuration of nitrogen and explain why it is found in period 2 and group 15 of the periodic table.

15 Determine the period and group of the elements with the following electron configurations.
- **a** $1s^2 2s^2$
- **b** $1s^2 2s^2 2p^6 3s^2 3p^2$
- **c** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^3$

16 Write an equation, including state symbols, for the first ionisation energy of aluminium.

17 Two elements and/or ions that have the same electron configurations are known as:
- **A** isoelectronic
- **B** effective nuclear charges
- **C** amphoteric
- **D** metalloids.

18 Oxygen can undergo which types of chemical bonding? (More than one answer may be correct.)
- **A** metallic
- **B** non-metallic
- **C** ionic
- **D** covalent

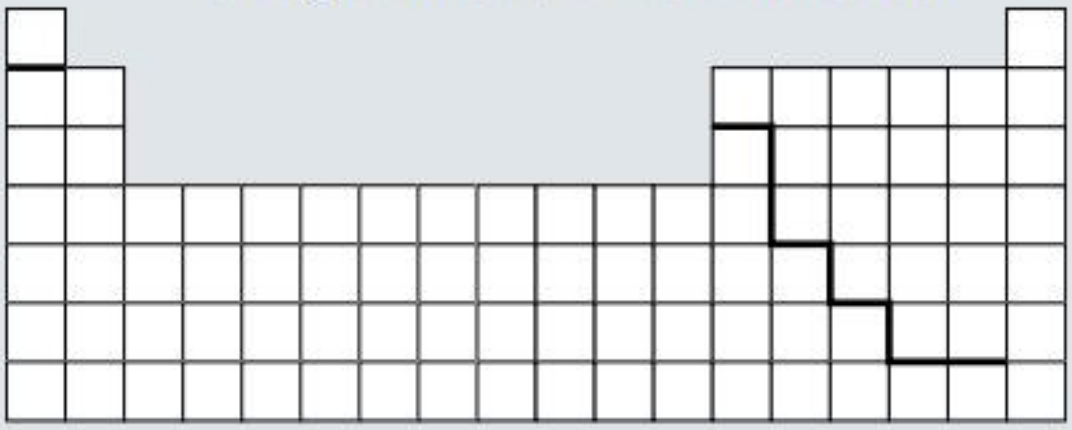
19 Explain each of the following briefly.
- **a** The atomic radius of chlorine is smaller than that of sodium.
- **b** The first ionisation energy of fluorine is higher than that of lithium.
- **c** There are two groups in the *s* block of the periodic table.

20 Explain the trend of ionic radii across a period.

21 Describe the changes that occur in the metallic character of the elements in period 2 of the periodic table.

22 Explain how you would expect each of the following properties to change based on effective nuclear charge and shielding.
- **a** electronegativity down a group
- **b** the radius of an anion compared to its parent atom

23 Use the blank periodic table below to identify and label the regions of metals, non-metals and metalloids.



24 Which of the following statements is incorrect?
- **A** Atomic radii of elements decrease across a period.
- **B** Electronegativity decreases across a period.
- **C** Metallic character decreases across a period.
- **D** First ionisation energy increases across a period.

Analyse

25 Identify the correct chemical symbol for each of the following using the periodic table in Figure 4.1.1 on page 50.
- **a** the element that is in group 2 and period 4
- **b** a noble gas with exactly three occupied electron shells
- **c** an element from group 14 that is a non-metal
- **d** an element that has exactly three occupied electron shells and is in the *s* block
- **e** the element in period 2 that has the largest atomic radius
- **f** the element in group 15 that has the highest first ionisation energy
- **g** the element in period 2 with the highest electronegativity

26 Determine the electron configuration of the following elements using the periodic table in Figure 4.1.1 on page 50.
- **a** phosphorus
- **b** Mg
- **c** element in period 4, group 14
- **d** element in period 2, group 16

27 Identify the group in the periodic table in which each of the following elements belongs. Use the periodic table in Figure 4.1.1 on page 50 as a reference.
- **a** B
- **b** Cl
- **c** Na
- **d** Ar
- **e** Si
- **f** Pb

28 Organise the following atoms in increasing atomic radius: Mg, Na, K, Ca.

29 Sort the following elements in order of increasing first ionisation energy: Mg, F, Na, K, Ca.

30 Use your knowledge of the trends in the periodic table to determine which element in each of the following sets has the largest first ionisation energy.

a phosphorus, arsenic, nitrogen

b sodium, potassium, calcium

c silicon, chlorine, sulfur

31 Identify which of the following pairs of elements would react together most vigorously.

Li and Cl_2; Li and Br_2; K and Cl_2; K and Br_2

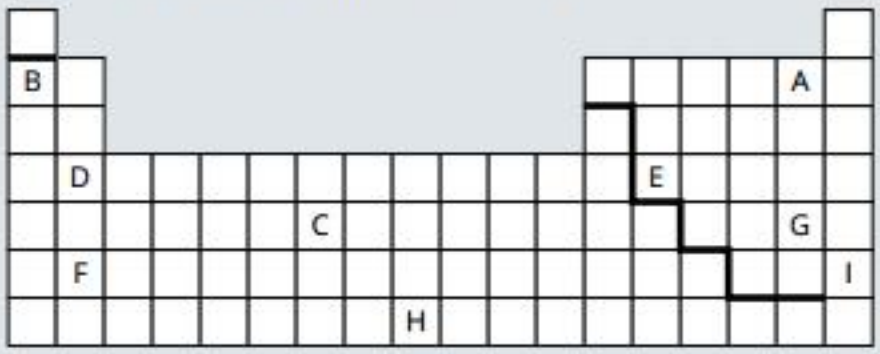
32 **a** Sort the following elements from least reactive to most reactive: rubidium, sodium, lithium, potassium.

b Explain your reasoning.

33 Predict the first ionisation energy of xenon using the information about first ionisation energies and atomic number of the noble gases in the following table.

Atomic number	First ionisation energy ($kJ\,mol^{-1}$)
2	2372
10	2081
18	1521
36	1351
54	

34 Identify the elements that meet the criteria below using the following hypothetical periodic table.



a have the same number of valence electrons

b are in the same period

c has smallest atomic radius

d has smallest ionic radius

e has lowest electronegativity

f is a noble gas

g is classified as a non-metal

h is classified as a metalloid

35 Predict the type of chemical bonding that magnesium can undergo.

36 An element has a first ionisation energy of $800\,kJ\,mol^{-1}$ and an electronegativity value of 2.0. Using the information in Figures 4.2.5 and 4.2.8 (pages 58 and 63), which of the following best describes this element?

A The element is in group 1 of the periodic table.

B The element is in group 3 of the periodic table.

C The element is in group 13 of the periodic table.

D The element is in group 17 of the periodic table.

37 Classify the oxides formed by the following elements as basic, amphoteric or acidic.

a magnesium

b phosphorus

c chlorine

d aluminium

38 Explain why the atomic radii of group 1 elements are larger than their ionic radii.

Interpret

39 Investigate the relationship between the metallic character of an element and its first ionisation energy.

Based on your findings, explain the variation of metallic character in relation to the position of the element in the periodic table.

40 Atomic radius, ionic radius, first ionisation energy, electronegativity and metallic properties all have trends as you move from left to right as well as from top to bottom on the periodic table. Summarise the key factors that determine these trends.

CHAPTER

05 Analytical techniques

Think about what you had for breakfast today. The packaging on any processed food you ate, including cereal, milk, bread and yoghurt, has a label that provides you with nutritional information, so you can make healthy diet choices. This information comes from chemical analysis.

Analytical chemists are employed in a range of industries, including food manufacturing, environmental monitoring, forensic sciences and many more. They use a range of techniques to determine the identity, quality and quantity of the chemicals that make up our world.

Analytical techniques allow us to characterise qualitatively (what is present) or quantitatively (how much is present) the composition of any material and its chemical state. In this chapter, you will look at techniques that involve the interaction of radiation with a material to provide us with information about:

- the types of element, isotope or compound that are present (qualitative analysis)
- how much of a particular element, isotope or compound is present (quantitative analysis).

Syllabus subject matter

Topic 1 • Properties and structure of atoms

ANALYTICAL TECHNIQUES

- State that mass spectrometry involves the ionisation of substances and the separation and detection of the resulting ions. (The operation of the mass spectrometer is not required.) **5.1**
- Analyse mass spectrometry spectra, to determine the isotopic composition of elements, the relative atomic mass of an element and percentage abundances of the isotopes of an element. **5.1**
- Discriminate between absorption and emission line spectra. **5.2**
- Explain that flame tests and atomic absorption spectroscopy (AAS) rely on electron transfer between atomic energy levels. **5.2**
- Explain that the emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels (Bohr model), which converge at higher energies. **5.2**
- Analyse flame tests and atomic absorption spectroscopy (AAS) to identify elements and determine the concentration of metallic ions in solution. **5.2**

ISOTOPES

- Explain that the relative atomic mass of an element is the ratio of the weighted average mass per atom of the naturally occurring form of the element to $\frac{1}{12}$ the mass of an atom of carbon-12. **5.1**

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5.1 Mass spectrometry

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that mass spectrometry involves the ionisation of substances and the separation and detection of the resulting ions, and that the spectra generated can be analysed to determine the isotopic composition of elements, and interpreted to determine the relative atomic mass
- use appropriate mathematical representations to make inferences and solve problems, including calculating the relative atomic mass of an element and percentage abundances of the isotopes of an element from data.

Mass spectrometry is one of the most common and useful analytical tools, as it can be used on its own or in combination with other techniques. In mass **spectrometry**, the substance that is being analysed interacts with **radiation**, which produces positive ions, resulting in a **mass spectrum**.

A **mass spectrometer** can be used for:

- **qualitative analysis**—to identify the unique fingerprint of a substance; this can then be used to identify the substance from an online database, to give information about the nature of the isotopes of elements present, or to determine the structure of a new or unknown compound
- **quantitative analysis**—as a sophisticated and very sensitive detector that can measure how much of a substance is present. This instrument can determine the masses of the isotopes of an element and their abundances; analysing this data from the mass spectrum allows you to calculate the relative atomic mass of each element.

All of this information can be determined using mass spectrometry. This module will focus on elemental analysis using mass spectrometry, as analysis of molecules is outside the scope of this unit.

MASSES OF PARTICLES

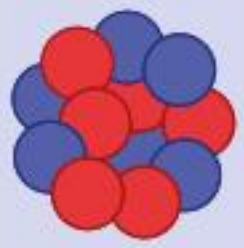
Since atoms are so small, it is not possible to determine their mass without specialised equipment. Scientists categorise the mass of the atoms in relation to a mole of the particles. A **mole** represents a fixed number of particles, 6.02×10^{23} to be precise. This will be covered in more detail in Chapter 9, but in this module, you will become familiar with the concepts of atomic mass and isotopic mass.

Relative isotopic mass

From Chapter 3, you will remember that **isotopes** are atoms of the same element that have different numbers of neutrons in their nuclei. So, isotopes have the same atomic number (number of protons) but a different mass number (number of protons plus neutrons).

The relative mass of an atom is based on a scale where the mass of a carbon-12 atom is exactly 12 units. Using this scale, the **relative isotopic mass** of an isotope is the mass of one atom of the isotope compared to one-twelfth of the mass of a carbon-12 atom. Table 5.1.1 shows the approximate relative isotopic mass of some isotopes.

TABLE 5.1.1 Approximate relative isotopic mass of some isotopes

Isotope	Diagram of nucleus	Number of protons in nucleus	Number of neutrons in nucleus	Total number of protons and neutrons	Approximate mass of atom relative to ^{12}C isotope
hydrogen $^{1}_{1}H$		1	0	1	$\frac{1}{12}$ of 12 = 1
helium $^{4}_{2}He$		2	2	4	$\frac{4}{12}$ of 12 = 4
lithium $^{7}_{3}Li$		3	4	7	$\frac{7}{12}$ of 12 = 7
carbon $^{12}_{6}C$		6	6	12	12

As shown in Figure 5.1.1, there are three different isotopes of the element magnesium:

- $^{24}_{12}Mg$, which contains 12 protons and 12 neutrons
- $^{25}_{12}Mg$, which contains 12 protons and 13 neutrons
- $^{26}_{12}Mg$, which contains 12 protons and 14 neutrons.

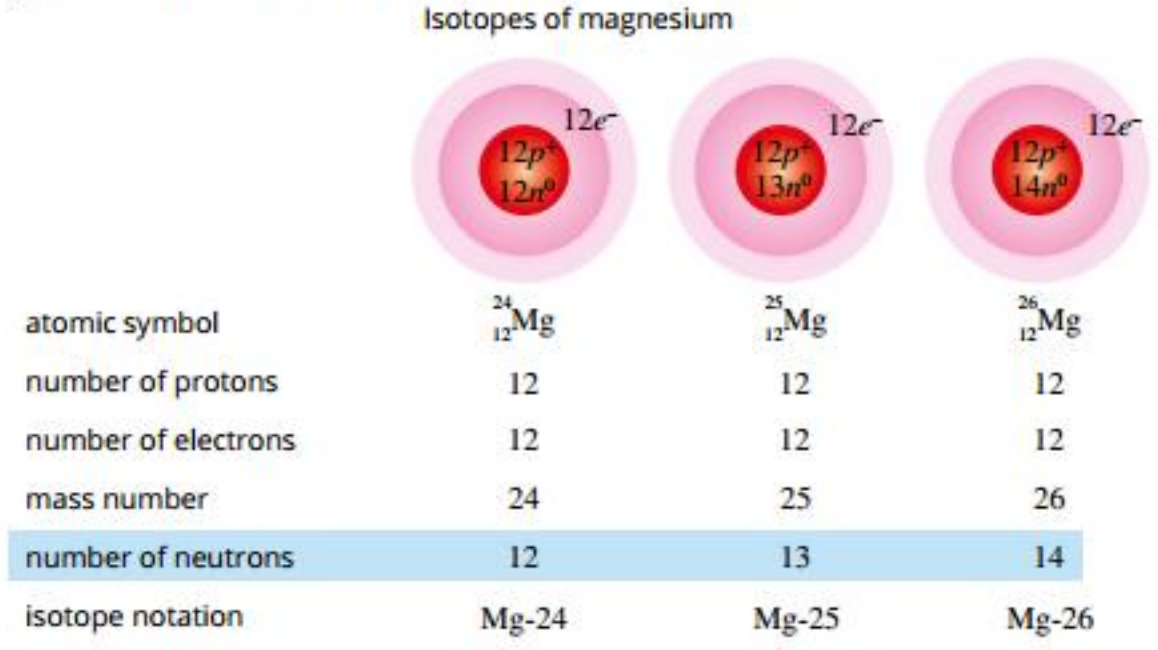


FIGURE 5.1.1 The three isotopes of the element magnesium. Different numbers of neutrons in the nuclei of these atoms give the atoms different masses.

The isotopes have different masses because they have different numbers of neutrons. Since the mass of an electron is relatively small, the mass of an atom is mainly determined by the mass of the protons and neutrons in its nucleus.

The relative isotopic masses of the three naturally occurring magnesium isotopes are experimentally determined to be 23.985 (^{24}Mg), 24.986 (^{25}Mg) and 25.983 (^{26}Mg). Since the masses of a proton and a neutron are similar and close to 1 on the $^{12}C = 12$ scale, the relative isotopic mass of an isotope is almost, but not exactly, equal to the number of protons plus neutrons in the nucleus.

The relative isotopic mass of an isotope is the mass of an atom of that isotope relative to the mass of an atom of carbon-12 (^{12}C) taken as 12 units exactly.

Relative isotopic abundance

Naturally occurring magnesium is made up of three isotopes, as shown in Figure 5.1.1, 78.99% of the lighter isotope and 10% and 11.01% of the two heavier isotopes, respectively. This composition is virtually the same no matter the source of the magnesium. The percentage abundance of an isotope in the naturally occurring element is called its **relative isotopic abundance**. Relative isotopic abundance is usually expressed as a percentage and is often called percentage abundance. Most elements, such as magnesium, are a mixture of two or more isotopes. Details of the isotopes of some common elements are shown in Table 5.1.2.

TABLE 5.1.2 Isotopic composition of some common elements

Element	Isotopes	Relative isotopic mass	Relative isotopic abundance (%)
hydrogen	^{1}H	1.008	99.986
	^{2}H	2.014	0.014
	^{3}H	3.016	0.0001
oxygen	^{16}O	15.995	99.76
	^{17}O	16.999	0.04
	^{18}O	17.999	0.20
silver	^{107}Ag	106.9	51.8
	^{109}Ag	108.9	48.2

THE MASS SPECTROMETER

Relative isotopic masses of elements and their **isotopic abundances** are determined by using an instrument called a mass spectrometer, which was invented by Francis Aston in 1919.

A mass spectrometer separates the individual isotopes in a sample of an element and determines the mass of each isotope, relative to the carbon-12 isotope, and the relative abundances of the isotopes.

Operation of a mass spectrometer

There are a number of different types of mass spectrometers; however, they work on similar basic principles. A diagram of a mass spectrometer is shown in Figure 5.1.2 and comprises several stages. While you are not required to learn how the mass spectrometer operates, it is important to understand these basic steps.

1 The sample is vaporised and the resultant gas is ionised to form positive ions.
2 The ions are then accelerated by an electric field.
3 These fast-moving ions are then separated by a magnetic field based on their mass-to-charge ratio.
4 The ions of a certain mass and charge reach a detector, which measures the current produced by a particular ion.

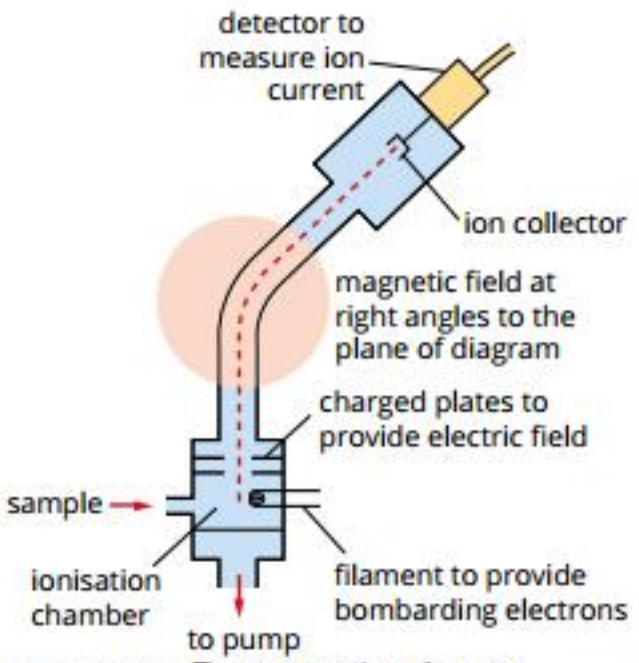

detector to measure ion current
ion collector
magnetic field at right angles to the plane of diagram
charged plates to provide electric field
sample
ionisation chamber
filament to provide bombarding electrons
to pump

FIGURE 5.1.2 The construction of a mass spectrometer. The sample is ionised and the ions pass through an electric field and a magnetic field before reaching the detector.

Mass spectra

The output obtained from a mass spectrometer is called a mass spectrum. Figure 5.1.3 shows the mass spectrum of magnesium.

- The number of peaks indicates the number of isotopes; in this case, three.
- The horizontal axis indicates the relative mass of each isotope present in an element according to the isotope's mass-to-charge ratio, which is given the symbol m/z or m/e. (The charge on most ions reaching the detector is +1, so the mass of an isotope can be read directly from the horizontal axis.) The three isotopes of magnesium have simplified relative masses of 24, 25 and 26. In fact, mass spectrometers can measure relative isotopic masses to an accuracy of three or more decimal places.
- The vertical axis indicates the abundance of each isotope in the sample; in this case, 79%, 10% and 11%.

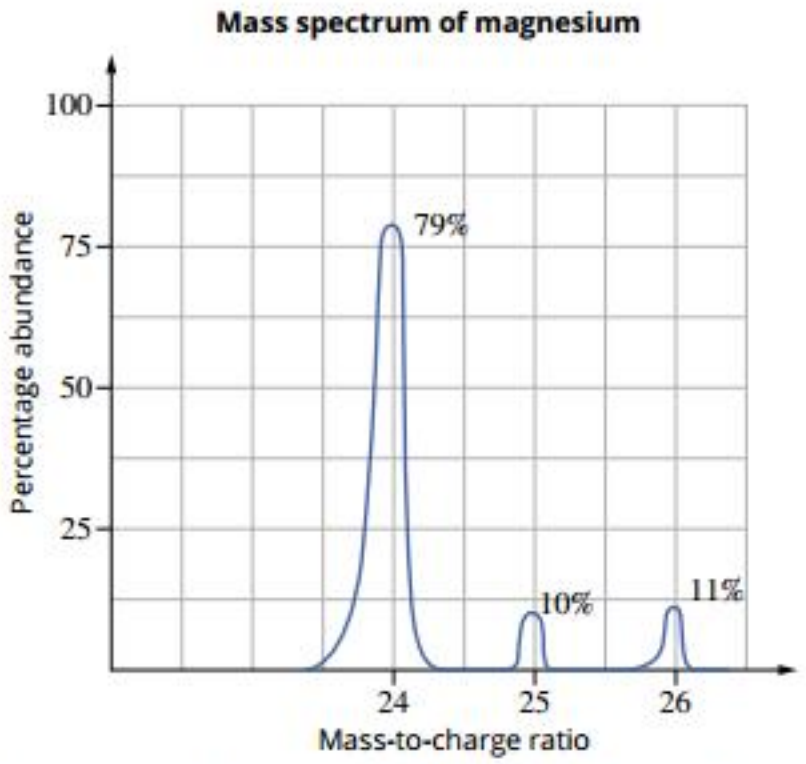


FIGURE 5.1.3 The mass spectrum of magnesium. The three peaks indicate there are three isotopes. The most abundant isotope has a relative isotopic mass of approximately 24 and an abundance of approximately 79%. The other isotopes have relative isotopic masses of approximately 25 and 26 and abundances of approximately 10% and 11%, respectively.

In summary, in the mass spectrum of an element, the:

- number of peaks indicates the number of isotopes
- position of each peak on the horizontal axis indicates the relative isotopic mass
- relative heights of the peaks correspond to the relative abundance of the isotopes.

RELATIVE ATOMIC MASS

Most elements consist of a mixture of isotopes. For the purpose of the calculations you will be doing later in this chapter, it is convenient to know the average relative mass of an atom in this mixture. This average is called the **relative atomic mass** of an element, and is given the symbol A_r.

The relative atomic mass is a weighted average based on the relative abundances of the isotopes that exist in a naturally occurring sample of the element. A more abundant isotope has a greater effect on the weighted average. Data obtained from the mass spectrum of magnesium shown in Figure 5.1.3 is summarised in Table 5.1.3.

The relative atomic mass of an element is the weighted average of the relative masses of the naturally occurring isotopes of the element on the ^{12}C scale.

TABLE 5.1.3 The isotopic composition of magnesium

Isotope	Relative isotopic mass	% abundance
^{24}Mg	23.985	78.99
^{25}Mg	24.986	10.00
^{26}Mg	25.983	11.01

The data about the three isotopes is used to calculate the relative atomic mass of magnesium, as shown in Worked example 5.1.1. Calculating the weighted average mass can be thought of as finding the mass of 100 atoms and then dividing by 100 to find the average mass per atom. The formula is shown below.

The relative atomic mass (A_r) of an element with three isotopes can be calculated using the formula:

$$A_r = \frac{(\text{relative isotopic mass} \times \% \text{ isotopic abundance})}{100} + \frac{(\text{relative isotopic mass} \times \% \text{ isotopic abundance})}{100} + \frac{(\text{relative isotopic mass} \times \% \text{ isotopic abundance})}{100}$$

The periodic table at the back of the book provides the relative atomic mass of each element.

Worked example 5.1.1

CALCULATING RELATIVE ATOMIC MASS FROM ISOTOPIC MASSES AND PERCENTAGE ABUNDANCES

Determine the relative atomic mass of magnesium from the data obtained from Table 5.1.3.

Thinking	Working
Determine the relative isotopic mass and abundance of each isotope.	The table shows three isotopes. First isotope: relative isotopic mass 23.985; abundance 78.99% Second isotope: relative isotopic mass 24.986; abundance 10.00% Third isotope: relative isotopic mass 25.983; abundance 11.01%
Substitute the relative isotopic masses and abundances into the formula for calculating relative atomic mass: $A_r = \frac{(\text{relative isotopic mass} \times \% \text{ isotopic abundance})}{100} + \frac{(\text{relative isotopic mass} \times \% \text{ isotopic abundance})}{100} + \frac{(\text{relative isotopic mass} \times \% \text{ isotopic abundance})}{100}$	$A_r = \frac{(23.985 \times 78.99) + (24.986 \times 10.00) + (25.983 \times 11.01)}{100}$
Calculate the relative atomic mass.	$A_r = \frac{1894.58 + 249.86 + 286.07}{100}$ $= 24.3051$
Express the answer to 2 decimal places.	$A_r(\text{Mg}) = 24.31$

➤ Try yourself 5.1.1

CALCULATING RELATIVE ATOMIC MASS FROM ISOTOPIC MASSES AND PERCENTAGE ABUNDANCES

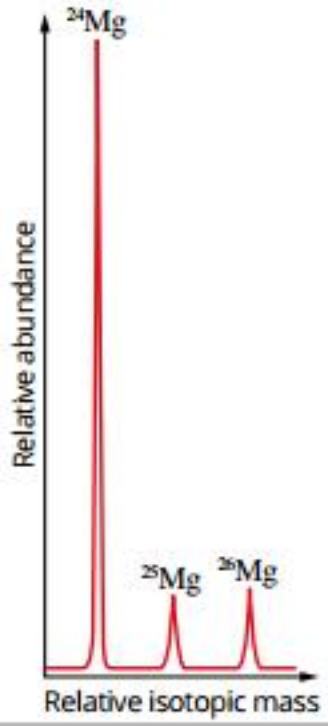
Boron has two isotopes. Their relative isotopic masses and percentage abundances are provided. Calculate the relative atomic mass of boron.

Isotope	Relative isotopic mass	% abundance
^{10}B	10.013	19.91
^{11}B	11.009	80.09

Worked example 5.1.2

CALCULATING PERCENTAGE ABUNDANCE OF EACH ISOTOPE FROM THE MASS SPECTRUM

Using the simplified mass spectrum of magnesium shown, calculate the percentage abundance of each of its three isotopes.

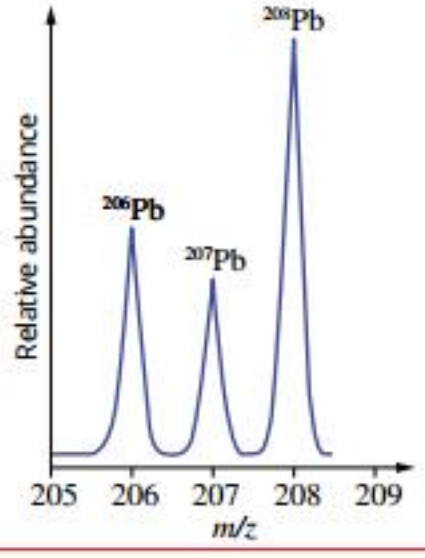


Thinking	Working
Measure the peak height for each isotope using a ruler.	From the spectrum, the height of each peak is: ^{24}Mg = 7.9 cm ^{25}Mg = 1.0 cm ^{26}Mg = 1.1 cm
Calculate the total peak height for the three isotopes by adding the individual peak heights.	Total peak height = 7.9 + 1.0 + 1.1 = 10 cm
Calculate each isotope's percentage abundance. This is the peak height as a percentage of the total peak height.	% abundance = $\frac{7.9}{10} \times 100 = 79\%$ % abundance = $\frac{1.0}{10} \times 100 = 10\%$ % abundance = $\frac{1.1}{10} \times 100 = 11\%$

➤ Try yourself 5.1.2

CALCULATING PERCENTAGE ABUNDANCE OF EACH ISOTOPE FROM THE MASS SPECTRUM

Using the simplified mass spectrum of lead shown, calculate the percentage abundance of each of its three isotopes.



Worked example 5.1.3

CALCULATING PERCENTAGE ABUNDANCES FROM RELATIVE ATOMIC MASS AND THE ISOTOPIC MASSES

The relative atomic mass of rubidium is 85.47. The isotopic masses of its two isotopes are 84.95 and 86.94. Calculate the relative abundances of the isotopes in naturally occurring rubidium.

Thinking	Working
State the relative abundances of the isotopes in terms of x, where x is the abundance of the lighter isotope. The abundance of lighter isotope is x. The abundance of heavier isotope must equal $100 - x$.	Abundance of 84.95 isotope = x Abundance of 86.94 isotope = $100 - x$
Substitute the isotopic masses, relative abundances and relative atomic mass into the formula: $A_r = \frac{(\text{isotopic mass} \times \% \text{ isotopic abundance})}{100} + \frac{(\text{isotopic mass} \times \% \text{ isotopic abundance})}{100}$	$85.47 = \frac{84.95x + (86.94 \times (100 - x))}{100}$
Expand the top line of the equation.	$85.47 = \frac{84.95x + 8694 - 86.94x}{100}$
Solve the equation to find x, the relative abundance of the lighter isotope.	$8547 = 84.95x + 8694 - 86.94x$ $8547 - 8694 = 84.95x - 86.94x$ $-147 = -1.99x$ $x = 73.87\%$ $= 73.9\%$
Determine the abundance of the heavier isotope.	Abundance of 86.94 isotope $= 100 - x$ $= 100 - 73.87$ $= 26.1\%$

➤ Try yourself 5.1.3

CALCULATING PERCENTAGE ABUNDANCES FROM RELATIVE ATOMIC MASS AND THE ISOTOPIC MASSES

The relative atomic mass of copper is 63.54. The isotopic masses of its two isotopes are 62.95 and 64.95. Calculate the relative abundances of the isotopes in naturally occurring copper.

5.1 Review

SUMMARY

- Most elements consist of a mixture of isotopes.
- The most common isotope of carbon, carbon-12, is used as the reference standard to compare the masses of atoms.
- The carbon-12 isotope is assigned a mass of exactly 12 units.
- The relative isotopic mass of an isotope is the mass of an atom of the isotope relative to the mass of an atom of carbon-12 taken as 12 units exactly.
- The relative isotopic mass and relative abundance of isotopes can be measured using a mass spectrometer.
- The relative atomic mass, A_r, of an element is a weighted average of its naturally occurring isotopic masses.
- Interpreting the mass spectrum of an element requires an understanding that:
  - the number of isotopes is equal to the number of peaks in the mass spectrum
  - the position of each peak on the horizontal axis indicates the relative isotopic mass
  - the abundance of isotopes is related to the relative heights of the peaks in the mass spectrum.

KEY QUESTIONS

Describe

1 **a** What is the atomic number of an element?
b Does the atomic number for atoms of the same element ever change?

2 Two atoms of magnesium have different masses.
a What feature of these atoms allows us to know they are both magnesium?
b Why do they have different masses?

3 Define the term 'isotope'.

4 Complete the table for the following isotopes.

Isotope name	Isotope symbol	Atomic number	Mass number	Number of protons	Number of neutrons	Number of electrons
		19	37			
oxygen-17			17			
uranium-235						
			238	92		
	$^{10}_{5}B$					
				5	6	

Apply

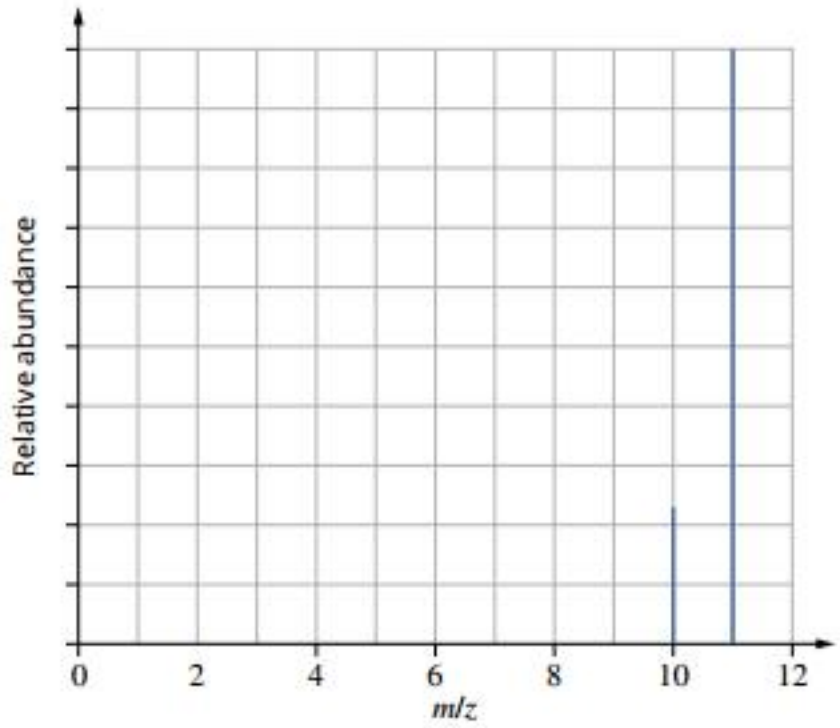
5 Explain what is separated and detected by mass spectrometers.

6 The atomic mass of magnesium (Mg) is given in the periodic table as 24.3, yet no single atom of magnesium has a mass of 24.3. Explain why.

Analyse

7 What is the number of protons, electrons and neutrons in a neutral atom of ^{37}Cl?

8 Calculate the relative atomic mass of the element shown in the following mass spectrum.



9 Calculate the number of protons, neutrons and electrons in each of the following ions.
a $^{63}_{29}Cu^{2+}$ **b** $^{14}_{7}N^{3-}$

10 The mass numbers of the two ions $^{54}_{26}Fe^{2+}$ and $^{56}_{26}Fe^{3+}$ are different. Is the difference in mass due to their two different charges? Explain.

11 Write the complete atomic symbol for an atom with the following characteristics.
a contains 19 electrons and 20 neutrons
b nitrogen atom with 8 neutrons
c bromine atom with a mass number of 80
d uranium atom with 146 neutrons
e copper atom with 65 nucleons

5.1 Review *continued*

12 A mass spectrum identifies three isotopes of iodine with isotopic abundances of 80% ^{127}I, 17% ^{126}I and 3% ^{128}I. Calculate the relative atomic mass of iodine.

13 Calculate the relative atomic mass of an element if 60.4% of the atoms have a mass of 68.9257 and the rest have a mass of 70.9249. Identify the element in the periodic table.

14 The table below includes some common elements and the relative abundance of a number of their isotopes.

Element	Isotope	Relative isotopic mass	Relative isotopic abundance
rubidium	^{85}Rb	84.911	72.17
	^{87}Rb	86.909	27.83
antimony	^{121}Sb	120.904	57.21
	^{123}Sb	122.904	42.79
strontium	^{84}Sr	83.913	0.56
	^{86}Sr	85.909	9.86
	^{87}Sr	86.909	7.00
	^{88}Sr	87.906	82.58
potassium	^{39}K	38.963	93.258
	^{40}K	39.964	0.0117
	^{41}K	40.962	6.7302
argon	^{36}Ar	35.968	0.3365
	^{38}Ar	37.963	0.0632
	^{40}Ar	39.962	99.6003

Calculate the relative atomic mass of the following elements using the information in the table.

a rubidium

b antimony

c strontium

15 Compare the relative atomic masses of argon and potassium using the isotopic data provided in the table in Question **14**. Would their relative positions in the periodic table change if the table were organised by atomic mass instead of atomic number?

16 The relative atomic mass of gallium is 69.723. The relative isotopic masses of its two isotopes are 68.926 and 70.925. Calculate the relative abundances of the isotopes in naturally occurring gallium.

17 Carbon has three isotopes and a relative atomic mass of 12.011. Given the following data, calculate the relative isotopic mass for carbon-13 to 5 significant figures.

Isotope	Relative isotopic mass	Relative abundance (%)
^{12}C	12.000	98.892
^{13}C		1.1080
^{14}C	14.003	2.0×10^{-10}

18 Why is tellurium placed before iodine in the periodic table when it has a higher relative atomic mass?

5.2 Atomic spectroscopy

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that flame tests (emission spectroscopy) and atomic absorption spectroscopy (AAS) are analytical techniques that can be used to identify elements. These methods involve interactions with radiation, so that electrons transition between atomic energy levels, causing the absorption or emission of energy. As a consequence, the spectra produced are line spectra, indicating the release (or absorption) of energy of a particular wavelength
- distinguish between absorption and emission spectra and recognise that the emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels (Bohr model), which converge at higher energies
- explain that emission spectra are produced when photons are emitted from atoms when excited electrons return to a lower energy level. The energy emitted is equal to the difference in energy between the two energy levels that electrons have moved between
- analyse, interpret and evaluate data from flame tests and atomic absorption spectrometry (AAS) to determine the presence and concentration of metallic ions in a solution.

You will be familiar with the colourful effects that are created in fireworks displays. Small quantities of different metal compounds are incorporated in fireworks to produce different colours. For example, in Figure 5.2.1, strontium compounds have produced the eye-catching scarlet colour and sodium compounds have produced the yellow. If you have ever spilt salt into the flame of a gas stove, you might have noticed this same yellow colour in the flame.

FIGURE 5.2.1 Metal compounds incorporated into fireworks are responsible for the colours in this display.

In Chapter 3, you explored the atomic structure of atoms. You learnt that electrons are arranged in shells at different distances from the nucleus. This was related to the energy possessed by each electron. In this module, you will apply your understanding to the identification of the elemental composition based on the colour of the light emitted from the excited species. In addition, you will examine how the emission and absorption of light by metals can be used to determine the concentration of salts in a solution.

SPECTROSCOPY

Spectroscopic techniques involve the interaction of compounds with radiation in different ways. The various techniques can be used for either qualitative or quantitative analysis. Techniques that are mainly used for qualitative analysis are called **spectroscopic techniques**, whereas those that are mainly used for quantitative analysis are called **spectrometric techniques**. In practice, some techniques can be used for both forms of analysis and the distinction between **spectroscopy** and spectrometry becomes blurred. In the case of mass spectrometry and **atomic absorption spectrometry**, which you will study, the techniques can be employed for both the identification of a material (qualitative analysis) and determination of composition (quantitative analysis). Indeed, the technique of atomic absorption spectrometry is often referred to as atomic absorption spectroscopy—with both using the same abbreviation, AAS.

Light is a form of energy and is a type of **electromagnetic radiation**. Other forms of electromagnetic radiation include radio waves and X-rays. Visible light is only a small part of the range of different forms of electromagnetic radiation. The **electromagnetic spectrum** (Figure 5.2.2) shows different types of radiation arranged according to their relative energies and **wavelengths** (the distance between peaks of the wave).

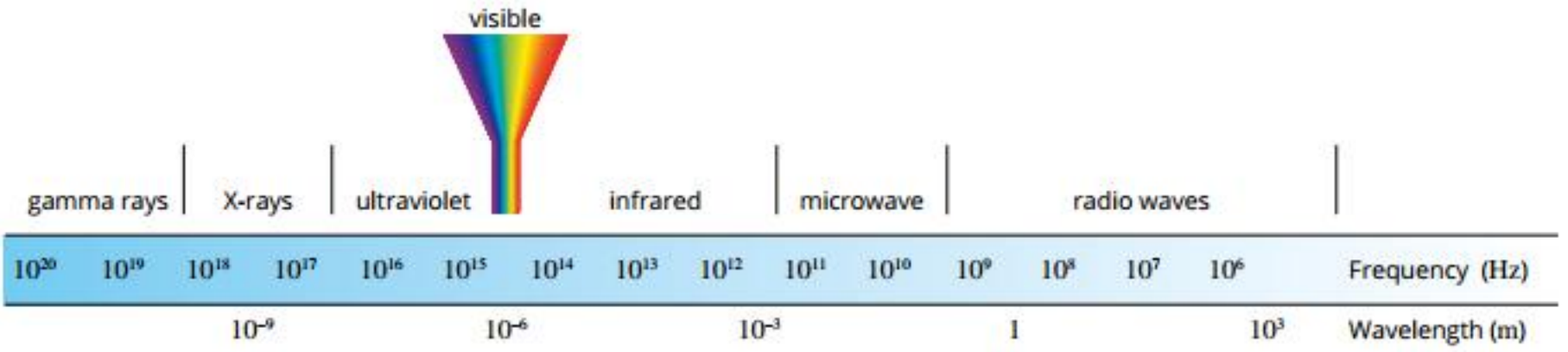


FIGURE 5.2.2 The electromagnetic spectrum. Visible light is only a small part of the electromagnetic spectrum. The analytical techniques detailed in this module use radiation within the visible spectrum.

i The visible spectrum of light corresponds to the radiation with wavelengths between 400 and 700 nm on the electromagnetic spectrum.

Electromagnetic radiation, such as light, can interact with atoms, and the nature of this interaction depends upon the energy of the electromagnetic radiation.

When a substance absorbs visible light, it appears coloured. The colour observed is not the same as the colour of the light absorbed. The colour you see is actually due to reflected or transmitted light. For example, plant leaves contain chlorophyll. When you look at the leaves, they appear green because chlorophyll absorbs light in the purple and red ranges of the spectrum. Chlorophyll does not absorb light in the green region of the spectrum, so this is reflected back into your eyes.

Spectroscopic techniques utilise the characteristics of atoms.

- Atoms absorb and emit electromagnetic radiation of specific energies.
- Atoms undergo a change when they absorb and emit electromagnetic radiation.
- Energy in different parts of the electromagnetic spectrum affects different parts of the atoms to different extents.
- The spectroscopic techniques that measure energy absorption are **absorption spectra** and the techniques that measure energy emission are **emission spectra**.

Radiation from each portion of the electromagnetic spectrum has a specific frequency, wavelength and energy associated with it. Ultraviolet light is very short wavelength radiation with high energy, while radio waves have long wavelengths and low energy.

The energy of the radiation determines which part of an atom is affected.

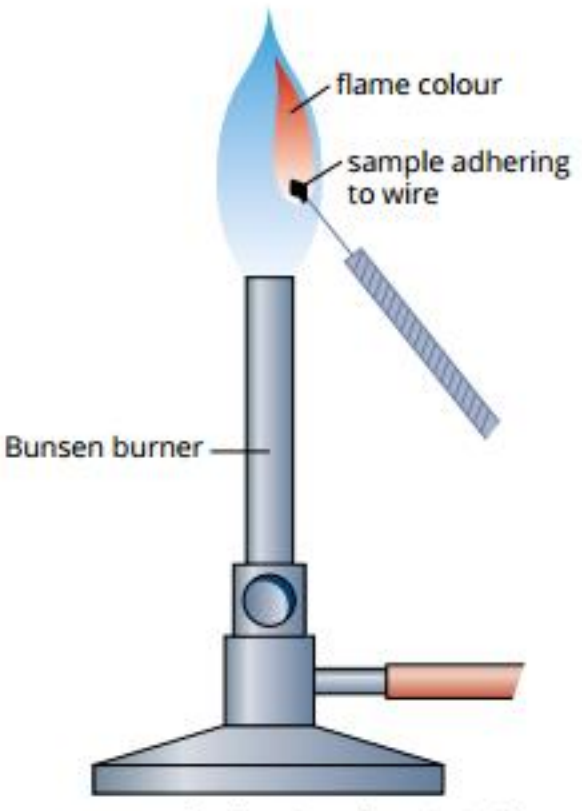


FIGURE 5.2.3 Performing a flame test. A moist wire has been dipped in the sample and then placed in the flame. A fine spray of solution from a spray bottle could be used instead.

FLAME TEST

Chemists use the fact that some metals produce particular colours when they are heated as a convenient and simple method of analysis. The metallic elements present in a compound can often be determined just by inserting a sample of the compound into a non-luminous Bunsen burner flame, as shown in Figure 5.2.3.

Most metal ions produce a characteristic colour when they are heated. This means that the metal in an unknown sample can be identified by comparing the flame colour with the known characteristic colours produced by metals. Some examples of the flame colours produced by metals can be seen in Figure 5.2.4.

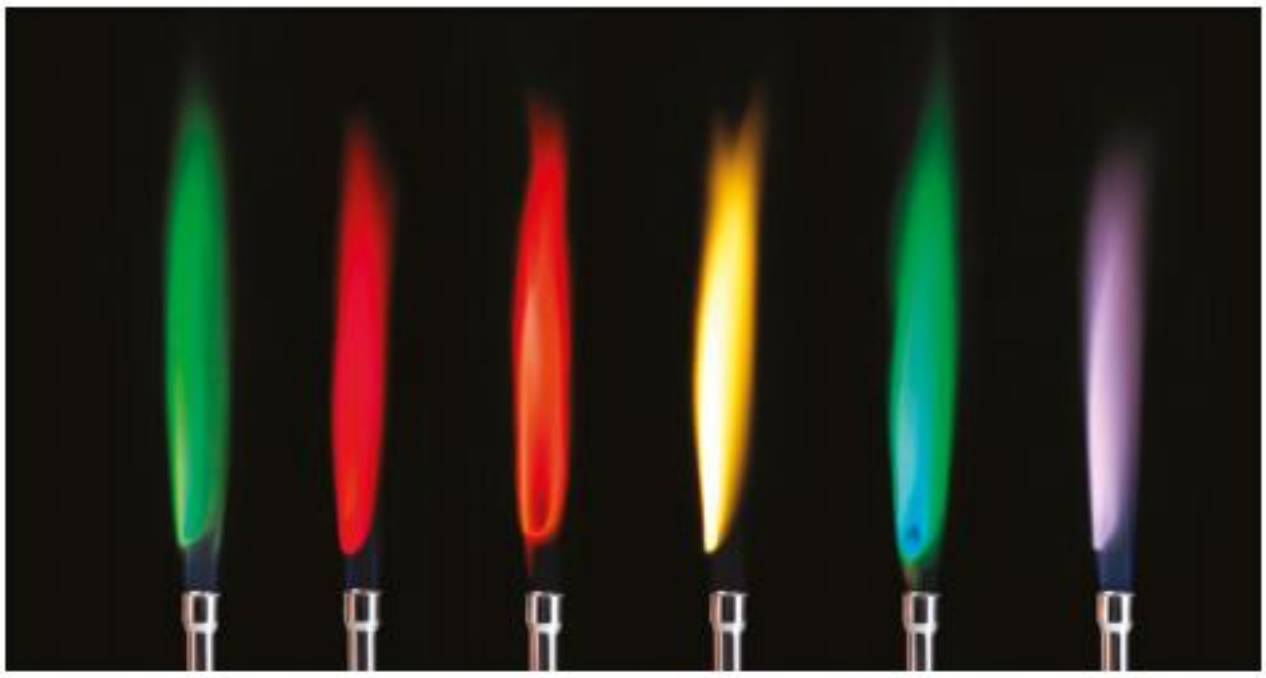


FIGURE 5.2.4 The colour of the flame is determined by the different metal compounds present and can be used to identify these metals. The flame colours shown here are for (from left to right) barium (yellow–green), lithium (crimson), strontium (scarlet), sodium (yellow), copper (green) and potassium (lilac).

Because each flame colour is unique, you can use the flame colour produced to qualitatively identify a metal ion in an unknown sample. Table 5.2.1 shows some of the flame colours that can be used to identify the presence of metals in a flame test.

TABLE 5.2.1 Characteristic flame colours of some metal ions

Metal	Flame colour
sodium	yellow
strontium	scarlet
copper	green
barium	yellow–green
lithium	crimson
calcium	yellow–red
potassium	lilac

It is important to note that only a small number of metals produce flame colours by this process. Although the exact colour produced by each metal is unique, simple flame tests can result in a level of uncertainty when trying to decide between different shades of similar colours such as scarlet (strontium), crimson (lithium) and yellow–red (calcium).

You will recall from Chapter 3 that electrons are arranged in atoms in different energy levels. Electrons in energy levels close to the nucleus have the lowest energies and experience the strongest attraction to the nucleus. When placed in a flame, an outer-shell electron can jump up to a higher energy level if it absorbs energy that corresponds exactly to the difference in energy between the lower energy level and the higher energy level (Figure 5.2.5).

Atoms with electrons in higher energy levels are unstable, so the **excited electrons** quickly return to lower energy levels. Figure 5.2.6 shows that the energy absorbed by the electrons is emitted as visible light when they return to a lower energy level.

When electrons are located in the lowest energy shells possible, the electrons are in the **ground state**.

If the energy emitted when electrons move from the higher energy level back to their original level falls within the region of the visible light spectrum, light of a specific colour is emitted (Figure 5.2.7). This emitted light is what you observe as the coloured flame in a flame test. The different colours observed correspond to specific wavelengths of light.

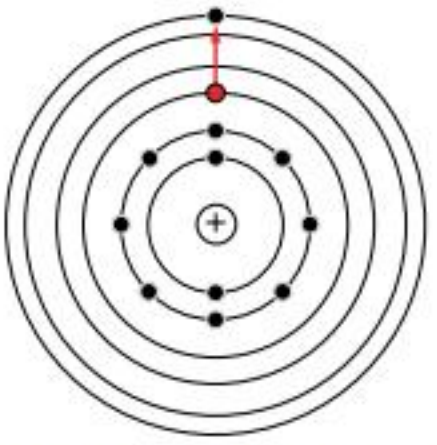


FIGURE 5.2.5 Energy from a flame can excite an electron in an atom to a higher energy level.

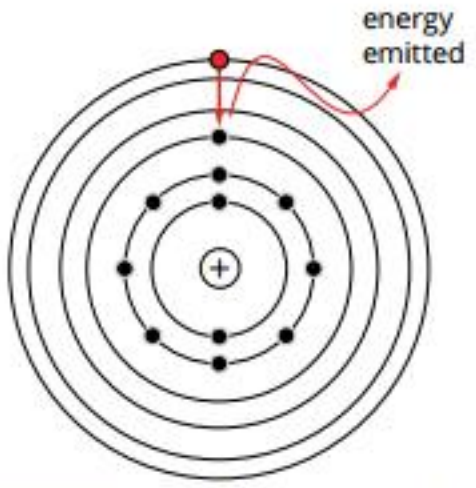


FIGURE 5.2.6 An excited electron quickly returns to a lower energy level, emitting electromagnetic energy in the form of visible light of a particular wavelength.

The colour of the light emitted from a sample is dependent on its energy. Red light has a lower energy than blue light.

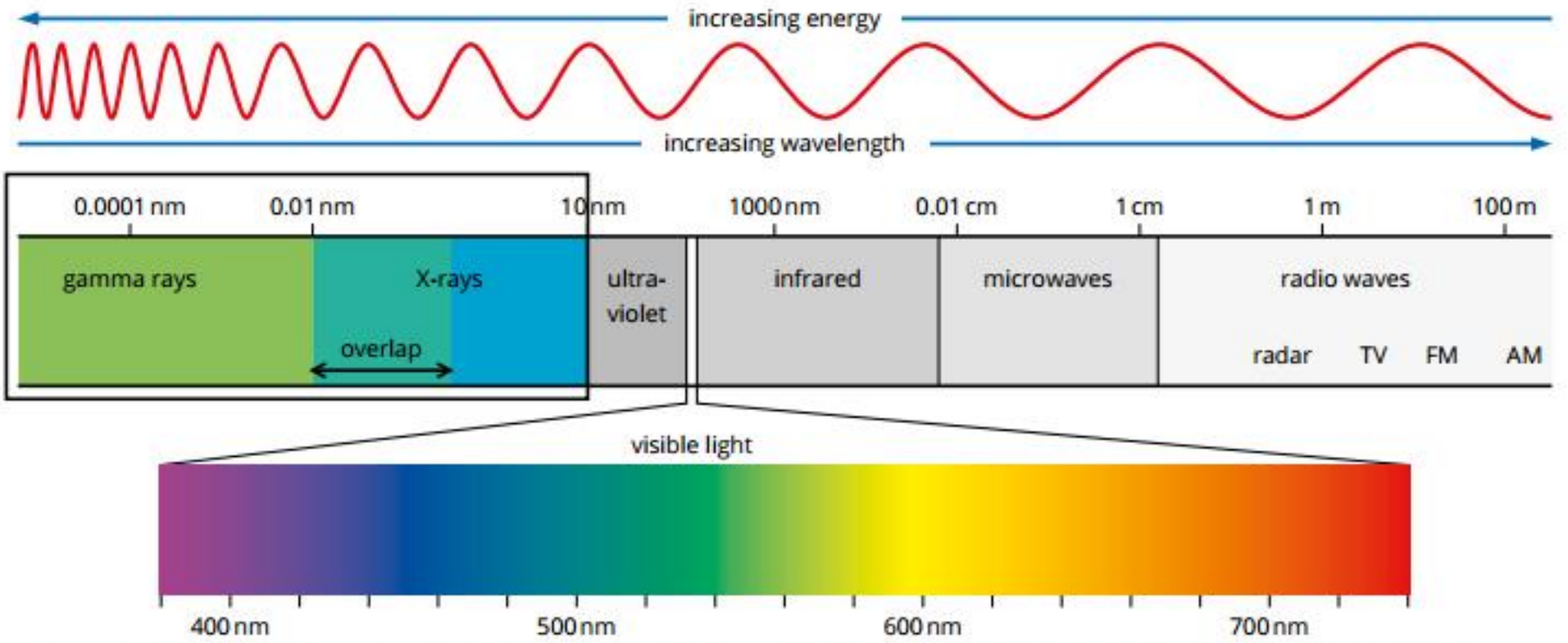


FIGURE 5.2.7 When excited electrons return to a ground state from a flame test, the emitted energy falls within the region of the electromagnetic spectrum that corresponds to visible light.

ATOMIC EMISSION SPECTROSCOPY

Flame tests provide only limited information about the likely elements present in a sample. As mentioned previously, only a few elements give a coloured flame in a Bunsen burner, and the colours of some are similar, which makes them difficult to tell apart. In impure samples, a faint colour may be masked by a stronger one. For example, the yellow emission from sodium ions is very strong, which means that it can overwhelm weaker colours, such as the lilac emission from potassium, so that a weaker colour, such as lilac, may not be visible in an impure sample.

An atomic emission spectrometer is an apparatus that can be used to determine the metal ions present in a sample (Figure 5.2.8). By making two changes to the flame test technique, the reliability and usefulness of flame colour identification is greatly improved.

- Using a hotter flame ensures that sufficient energy is available to excite electrons in a wider range of elements.
- Passing the light through a prism separates the different energies in the light emitted by a heated sample into a series of coloured lines called a **line spectrum** or an emission spectrum.

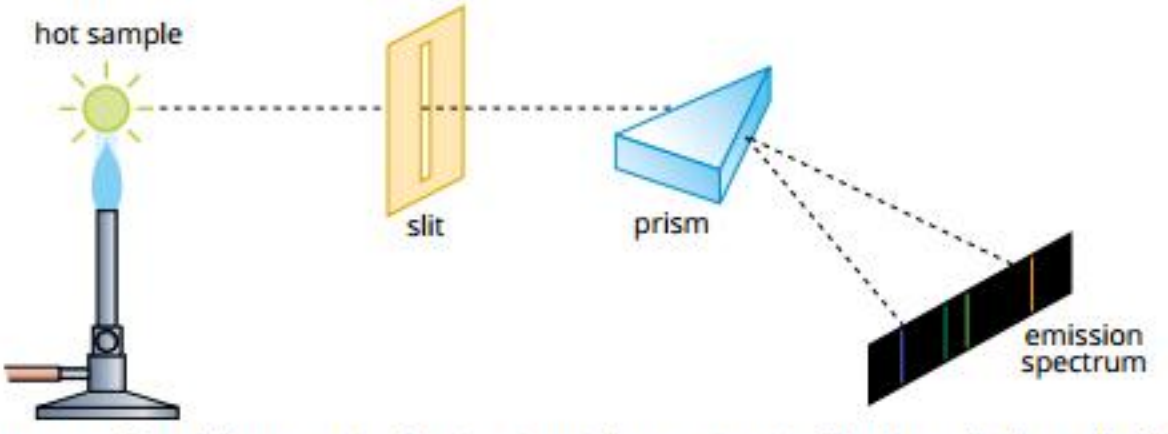


FIGURE 5.2.8 Essential components of an atomic emission spectrometer. The prism splits the emitted light into each of its component wavelengths, creating a line spectrum that is unique to the sample being tested.

When the light emitted from an excited atom is viewed through a spectrometer, it is much easier to see how the colour produced is unique. Because each element has a different number of protons in the nucleus and a unique electron configuration, the energy transitions that the electrons undergo as they move from the ground state to an excited state are also unique.

Therefore, no two elements have energy levels of exactly the same energy, so a spectrum is a characteristic of a particular element. It may be used as a 'fingerprint' to identify the elements present in a substance. The emission spectra of calcium, sodium, mercury and cadmium are shown in Figure 5.2.9 as examples. You can see how the spectra consist of distinct lines corresponding to the different colours emitted by the atoms. A particular element will always produce the same spectrum, meaning that the electrons of that element are only emitting those discrete amounts of energy. This provides evidence for the existence of electrons in discrete energy levels.

FIGURE 5.2.9 The emission spectrum of (a) calcium, (b) sodium, (c) mercury and (d) cadmium. The spectral lines are indicative of the different energies of light emitted in the visible region.

Formation of different spectral lines

Earlier in this module, you learnt that when unstable excited electrons in higher energy levels fall back to lower energy levels, they emit energy as light. When falling back to the same shell, an electron from a higher energy level emits more energy, which corresponds to light of a lower wavelength, compared to an electron that falls from a lower energy shell. For example, in a hydrogen atom, when an electron falls from $n = 3$ shell back to $n = 1$, it emits a photon with 12.09 eV (102.57 nm) compared to an electron that falls from $n = 2$ shell back to $n = 1$ and emits a photon with 10.20 eV (121.57 nm).

In the early 20th century, a series of spectral lines was observed in the hydrogen spectrum. The lines are grouped together in a series. There are several series of spectral lines, showing specific energy level spectrums. You can see in Figure 5.2.10 that, in the Balmer series of hydrogen, these lines get closer together until a **continuum** occurs. This indicates that the differences between each transition become less and less until they are indistinguishable from one another.

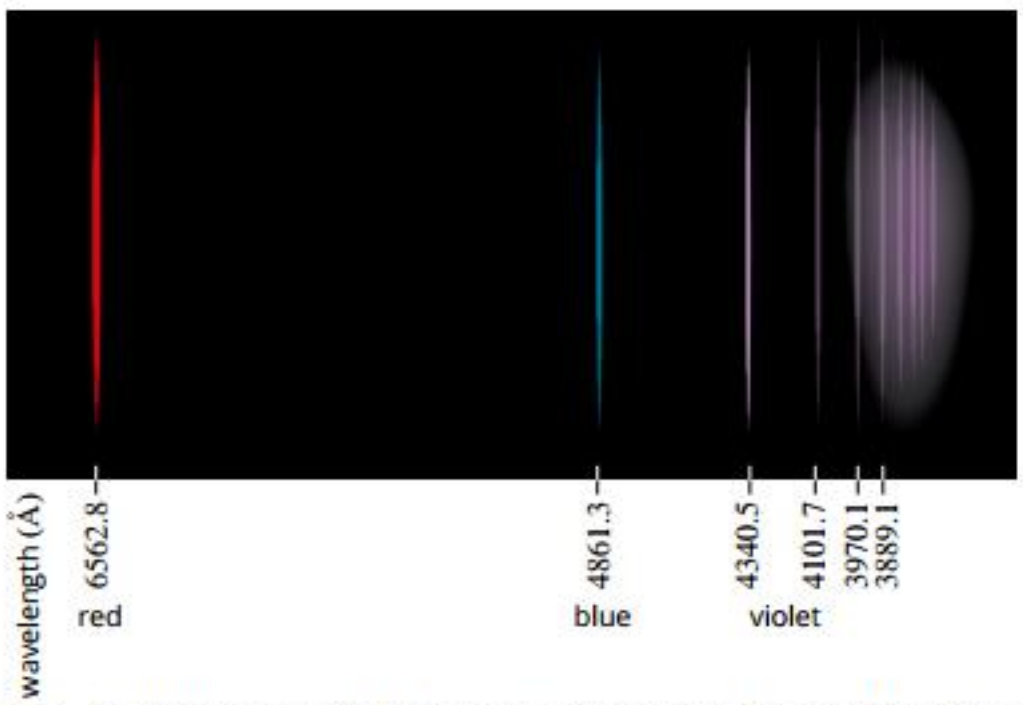


FIGURE 5.2.10 The electron transitions that create the Balmer series of spectral lines (in the visible spectrum) for the hydrogen atom

The series of lines observed corresponded to the energy levels to which the electrons returned. Electrons that fall back to the $n = 1$ shell are part of the **Lyman series** (ultraviolet). Emission lines produced from electrons that fall back to the $n = 2$ shell are known as the **Balmer series** (visible), and the **Paschen series** (infrared) corresponds to the spectral series in which electrons fall back to the $n = 3$ shell. So, all transitions from higher energy levels to the $n = 1$ shell result in lines in the ultraviolet region, all transitions to the $n = 2$ shell result in visible lines, and all transitions to the $n = 3$ shell result in infrared lines. The formation of the Lyman, Balmer and Paschen series of lines for the hydrogen atom is shown in Figure 5.2.11. There are additional spectral lines corresponding to higher energy shells ($n = 4$ and $n = 5$), but these are outside the scope of this course.

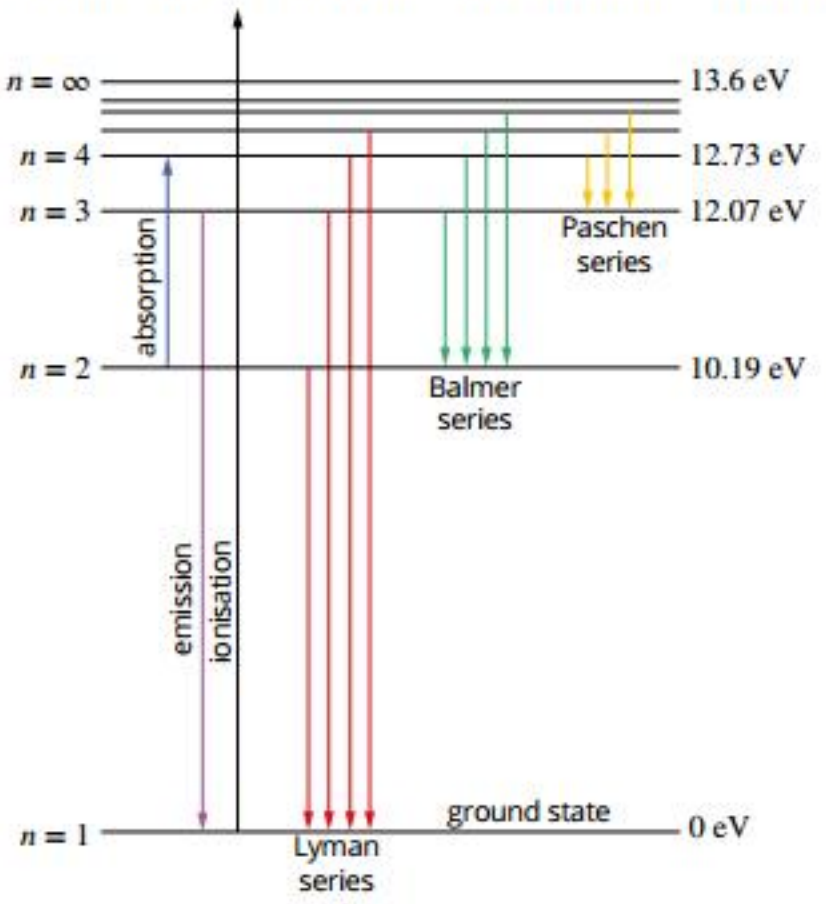


FIGURE 5.2.11 The electron transitions that create the Lyman, Balmer and Paschen series of spectral lines for the hydrogen atom. The differences between emission, absorption and ionisation are also shown.

ATOMIC ABSORPTION SPECTROMETRY

As you have seen, an emission spectrum occurs when energy is emitted as electrons move from a higher energy level to a lower energy level. The energy emitted is equal to the difference in energy between the two energy levels. Absorption is the opposite. When electrons absorb energy, if the amount of energy absorbed is equal to the difference in energy between one energy level and the next highest level, it will cause the electron to jump to that higher energy level.

In the early 1950s, Australian scientist Alan Walsh was working on the measurement of small concentrations of metals at the Commonwealth Scientific and Industrial Research Organisation (CSIRO). At this time, the technique of absorption spectroscopy was used for molecules and emission spectroscopy for atoms (elements). Alan Walsh realised the advantages of **atomic absorption spectroscopy (AAS)**, which is now used widely for detecting the presence of most metals and determining their concentration. He developed the atomic absorption spectrometer to carry out spectrometric (i.e. quantitative) analysis of metal concentrations in solutions.

How AAS works

Alan Walsh's breakthrough was to recognise that atoms will absorb light if the energy of the light is exactly equal to the energy required to promote an electron from its ground-state energy level to a higher energy level. As described for emission spectroscopy, every element absorbs light of different energies (and hence different wavelengths), which means that the amount of light absorbed by a sample at a specific wavelength can be used to determine the concentration of that element.

Unlike emission spectroscopy, AAS measures the amount of light *absorbed* by the sample.

Figure 5.2.12 gives a simplified depiction of how an atomic absorption spectrometer works.

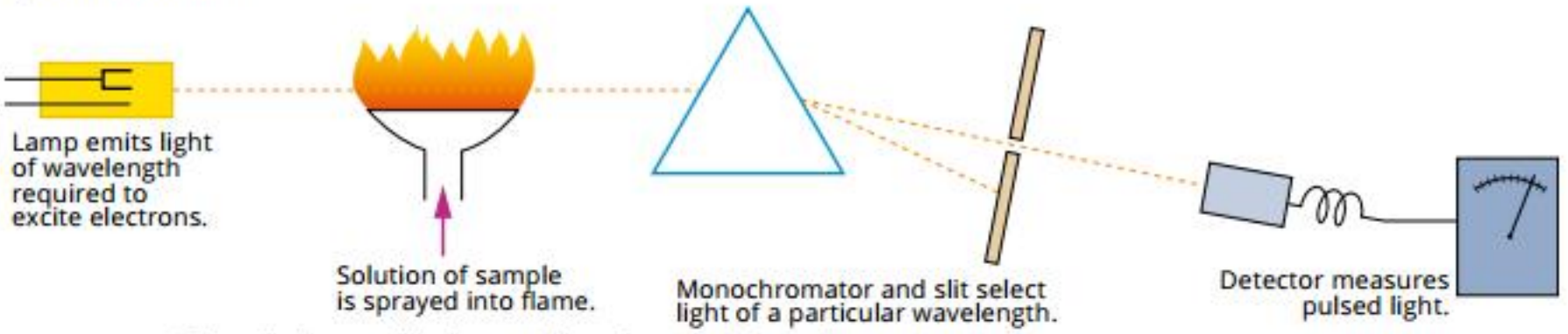

Lamp emits light of wavelength required to excite electrons.
Solution of sample is sprayed into flame.
Monochromator and slit select light of a particular wavelength.
Detector measures pulsed light.

FIGURE 5.2.12 Schematic diagram of the inner workings of an atomic absorption spectrometer.

The light absorbed at a specific wavelength by a sample can be determined by the following process.

1 A hollow cathode lamp emits different wavelengths of light that are absorbed by the metal being analysed. The lamp must be made with a filament of the metal being analysed.
2 A solution of the sample is sprayed into a flame to create an atomic vapour.
3 A monochromator is used to select a wavelength of light for analysis.
4 A detector measures the amount of light that reaches it, and a computer determines the amount of light that has been absorbed by the sample.

Comparing absorption and emission spectra

Figure 5.2.13 shows emission and absorption spectra from the analysis of hydrogen. They show evidence of the same electron transitions. The absorption spectrum shows the energy that is absorbed as electrons transition to a higher energy state. The emission spectrum shows the same energy that is released as the electrons return to a ground state. This is summarised in Figure 5.2.14.

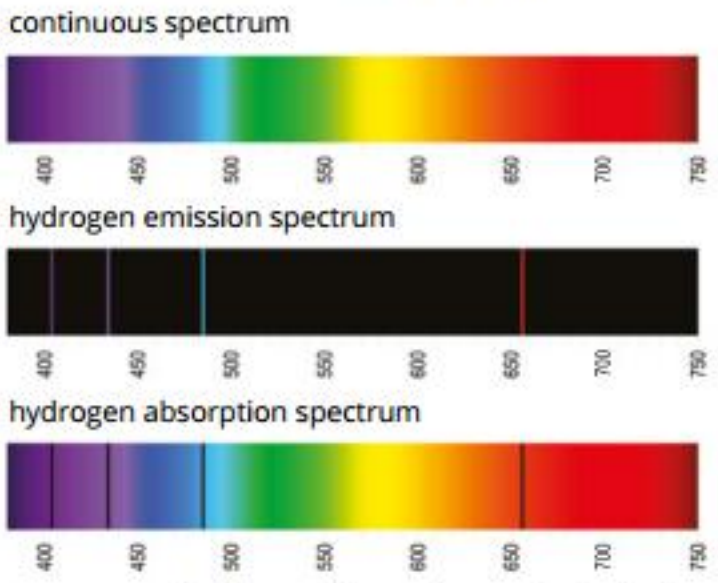


FIGURE 5.2.13 Emission and absorption spectra for hydrogen

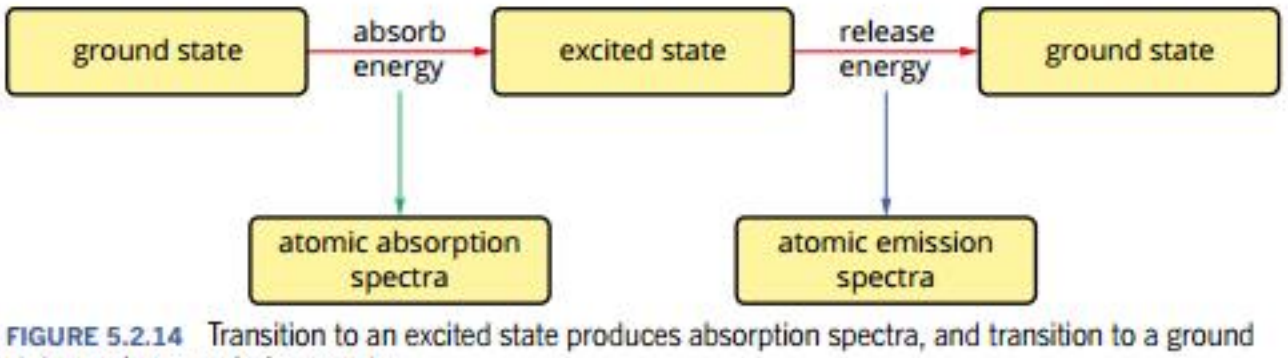


FIGURE 5.2.14 Transition to an excited state produces absorption spectra, and transition to a ground state produces emission spectra.

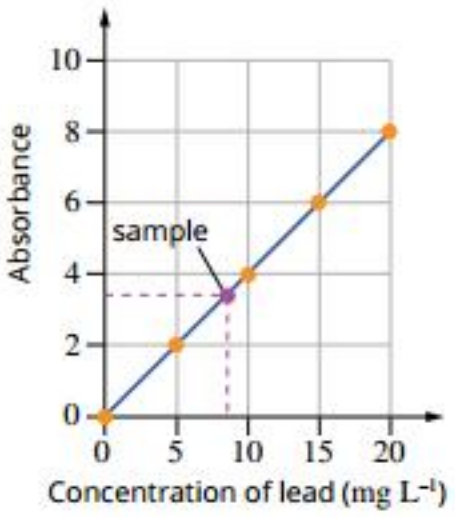


FIGURE 5.2.15 The AAS calibration curve shows the relationship between the absorbance of light and the concentration of lead in a sample.

As the concentration of the metal in the sample increases, the amount of light absorbed by the sample increases.

Calibration curves

Atomic absorption spectrometry can be used to simply detect the presence of most metals; however, it is more often used to determine the concentration of a metal in a sample. The absorbance measured for a sample can be related to the concentration of the metal being analysed by using a **calibration curve**.

To construct a calibration curve, you must first create a series of **standard solutions** of the metal ion (solutions of known concentration), and then measure their absorbance by AAS. A calibration curve is then constructed by accurately plotting the concentrations of the standard solutions against the absorbance of each solution, as shown in Figure 5.2.15.

Because the amount of light that is absorbed by the sample is proportional to the amount of metal present, the relationship between concentration and absorbance is a linear one.

Once constructed, the calibration curve can be used to determine the concentration of the metal being analysed in the unknown sample. The absorbance of the unknown sample is measured and the corresponding concentration value can be read from the graph.

There are many different units for concentration. For simplicity, concentration will be measured in $mg\,L^{-1}$ in the following examples, but it is important to always check the concentration unit specified on the x-axis of the calibration curve when answering questions involving AAS. In the example in Figure 5.2.15, the unit $mg\,L^{-1}$ refers to the mass of metal (in mg) in every litre of the solution being analysed.

Worked example 5.2.1

USING A CALIBRATION CURVE TO DETERMINE CONCENTRATION

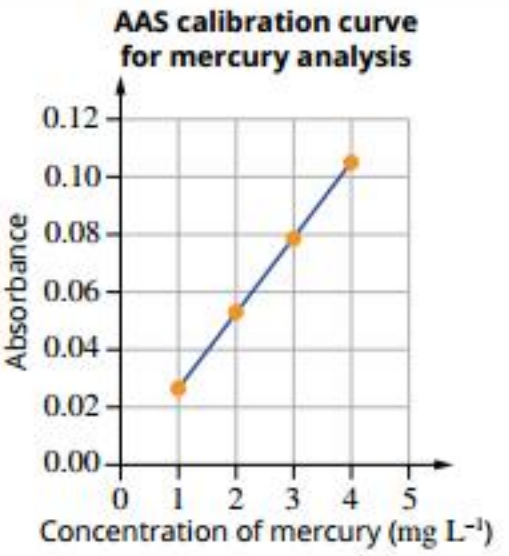
Determine the concentration of mercury in a sample, given the data in the following table.

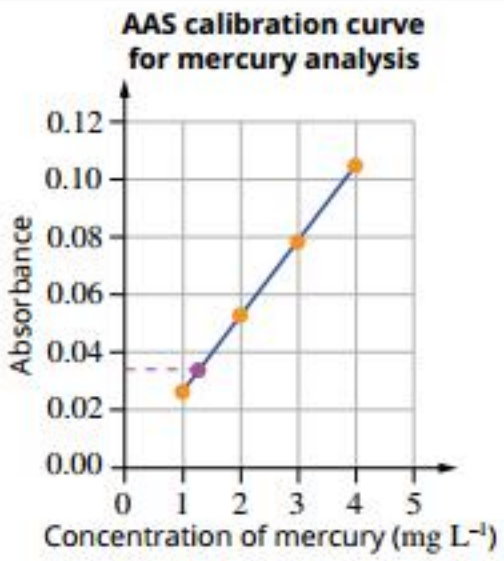
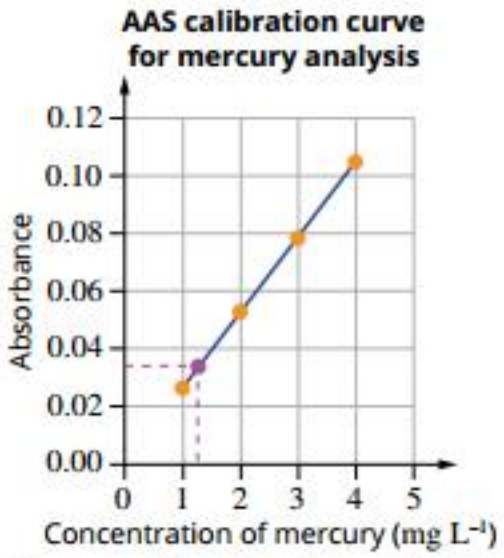
Concentration of mercury ($mg\,L^{-1}$)	Absorbance
1.0	0.026
2.0	0.053
3.0	0.078
4.0	0.105
sample	0.036

Thinking

Construct a calibration curve using concentrations of the standard solutions and their absorbance.

Working



Mark where the absorbance of the sample lies on the calibration curve. This can be done by finding the absorbance of the sample on the *y*-axis and moving horizontally right until you reach the calibration curve and marking that point.	
Determine the concentration of the sample by reading off the graph on the *x*-axis at the point where the sample's absorbance lies on the calibration curve.	 The sample's absorbance is 0.036. The concentration of mercury in the sample can be read from the graph as 1.2 mg L^{-1}.

➤ Try yourself 5.2.1

USING A CALIBRATION CURVE TO DETERMINE CONCENTRATION

Determine the concentration of sodium in a sample, given the data in the following table.

Concentration of sodium (mg L^{-1})	Absorbance
20	0.041
40	0.080
60	0.121
80	0.159
sample	0.104

AAS today

Approximately 60 years after Alan Walsh developed AAS, the technique is still being used by many modern-day chemists. It is a very good tool for analysing the concentration of metals in a wide variety of samples, including water, urine, blood, soil, fish and other foods. AAS is capable of detecting 68 different metallic elements, and is sensitive enough to detect metals present in concentrations of less than 1 mg L^{-1}.

Figure 5.2.16 shows an analytical chemist using an atomic absorption spectrometer to analyse the concentration of potassium in a sample.

FIGURE 5.2.16 An analytical chemist using AAS to determine the concentration of metals in food samples.

ICP–AES analysis

Even with the use of very hot flames (a mixture of oxygen and ethyne gas gives the hottest flame, up to 3100°C), there are still many elements that cannot be analysed by AAS or give a poor response.

Modern instruments, such as that seen in Figure 5.2.17, can analyse most elements by using an energy source called **inductively coupled plasma (ICP)** in combination with atomic emission spectroscopy (AES). Instead of a flame to excite the atoms, the ICP generates very high temperatures of up to 10 000°C to create a **plasma**, a state of matter containing charged particles. At these temperatures, virtually all the atoms in the sample are excited and are able to emit electromagnetic radiation as an emission spectrum as they return to their ground state, and only a very small quantity of an element needs to be present in order for it to be detected.

FIGURE 5.2.17 An ICP atomic emission spectrometer

5.2 Review

SUMMARY

- An atom in which the electrons are in their lowest possible energy state is said to be in its ground state.
- When an element is heated, outer-shell electrons may absorb energy and move into higher energy levels (shells). The atom is described as being excited.
- When the electrons move back to lower energy levels, they emit electromagnetic radiation, such as light, with specific energies; each element emits light with a unique set of energies called an emission spectrum.
- The shell to which the electron returns determines the spectral series associated with the light emission. For the hydrogen atom, if electrons from higher energy levels return to energy level $n = 1$, the emission of energy is part of the Lyman series (ultraviolet); if electrons return to energy level $n = 2$, the emission is part of the Balmer series (visible); and if electrons return to energy level $n = 3$, the emission is part of the Paschen series (infrared).
- Flame tests are performed by inserting a sample in a non-luminous Bunsen burner flame.
- Flame tests can be used to detect the presence of a small number of metal elements.
- The accuracy of flame tests is hampered by our ability to detect small differences in colours.
- Emission spectra are unique for each element and represent each of the energy transitions within an element as a series of different-coloured lines.
- The techniques of atomic absorption spectroscopy and spectrometry (AAS) are based on the ability of electrons to absorb a specific amount of energy as they move to higher energy levels.
- Atomic absorption spectrometry can be used to accurately determine the concentration of most metals in samples of water and other substances.
- The atomic absorption spectrometry technique involves the construction of a calibration curve to relate the concentration of the metal to the absorbance measured.

KEY QUESTIONS

Describe

1 What range of wavelengths of light are in the visible region of the electromagnetic spectrum?

2 Select words from the following list to complete the sentences below. Not all of the words provided are required.

protons, higher, transition, electrons, lower, let out, emit, excited

When a sample containing copper is heated in the flame of a Bunsen burner, the flame turns green. This is because the _____ in the copper atoms absorb energy and move to _____ energy levels and then _____ light that corresponds to a green colour as they return to _____ energy levels.

3 Name the first three spectral series for the hydrogen atom and the region in the emission spectrum where this electromagnetic radiation is observed.

Apply

4 With reference to electrons moving between energy levels, explain the differences between absorption of energy and emission of energy.

5 Consider the Balmer series of spectral lines in the emission spectrum of hydrogen, shown in Figure 5.2.10. Briefly explain how this spectrum provides evidence for the existence of electrons in discrete energy levels.

6 Flame colours could be used to quickly determine the presence of a particular metal in the following samples. For each case below, would this technique always give clear results? Explain.

a sodium fluoride in toothpaste

b sodium chloride in seawater

c strontium and calcium in dairy products

d potassium in mineral water

Analyse

7 A student observed the results shown in the table below from a flame test experiment. Using the characteristic flame colours shown in Table 5.2.1 on page 91, analyse these results, identify any anomalies and suggest a reason for any differences.

Metal	Flame colour
sodium	yellow
strontium	yellow
copper	green
lithium	crimson

5.2 Review *continued*

8 Figure 5.2.3 on page 90 shows a flame test being performed.

- **a** Identify what colour the flame would be if copper were present in the sample.
- **b** Deduce why it is necessary to heat the wire strongly for several minutes before performing the test.
- **c** Explain why copper wire would be unsuitable for use in flame tests.
- **d** Explain why flame tests are rarely used for qualitative analysis by modern chemists.

9 The following statement was written by a Chemistry student in a test. Correct the student's answer, and analyse the errors.

When potassium chloride is spilled into a gas flame, the flame turns bright yellow. The colour is due to electrons releasing energy as they move from a lower energy level to a higher energy level.

10 Determine whether light energy is emitted or absorbed when an electron goes from energy level $n = 5$ to $n = 2$.

11 Evaluate why atomic emission spectroscopy (AES) is regarded as a superior method of analysis to flame tests.

12 **a** Plot a calibration curve using the absorbance readings of the standard solutions containing potassium ions given below.

Concentration of potassium ($mg\,L^{-1}$)	Absorbance
0.0	0.01
2.0	0.08
4.0	0.15
6.0	0.21
8.0	0.27

- **b** Use the calibration curve you created in part **a** to determine the concentration of potassium, in $mg\,L^{-1}$, in a sample solution that gives an absorbance of 0.17.

13 Iron is essential to our health. To determine the iron content in a Milo milk drink, a 5.0 mL sample was diluted to 50.0 mL. The absorption of the diluted solution and several standard solutions was measured using AAS. The results are shown in the following table.

Solution concentration (ppm)	Absorbance
0.00	0.010
1.00	0.080
2.00	0.150
3.00	0.220
4.00	0.290
sample	0.185

- **a** Plot a graph of absorbance against concentration of iron.
- **b** Calculate the concentration of iron, in ppm, in the diluted Milo (1 ppm is 1 g iron per 10^6 g of Milo).
- **c** Calculate the concentration of iron, in ppm, in the undiluted Milo.
- **d** Determine the mass of iron you would consume by drinking a 250 mL glass of Milo (assume 1 mL = 1 g).
- **e** The recommended daily allowance (RDA) of iron for people over the age of 11 years is 18 mg. Calculate the percentage of your RDA that a 250-mL glass of Milo provides.
- **f** The 0.00 ppm standard, which contained no added iron, gave a small absorbance reading. Suggest an explanation for this.
- **g** Suggest why the sample of Milo was diluted to measure its absorbance.

Chapter review

05

KEY TERMS

absorption spectrum
atomic absorption spectrometry (AAS)
atomic absorption spectroscopy (AAS)
Balmer series
calibration curve
continuum
electromagnetic radiation
electromagnetic spectrum
emission spectrum
excited electron
ground state
inductively coupled plasma (ICP)
isotope
isotopic abundance
line spectrum
Lyman series
mass spectrometer
mass spectrum
mole
Paschen series
plasma
qualitative analysis
quantitative analysis
radiation
relative atomic mass
relative isotopic abundance
relative isotopic mass
spectrometric technique
spectroscopic technique
spectrometry
spectroscopy
standard solution
wavelength

KEY QUESTIONS

Describe

1 An element has the following three isotopes: $^{12}_{6}X$, $^{13}_{6}X$, $^{14}_{6}X$.
- **a** Identify the element.
- **b** What do the numbers 12, 13 and 14 refer to?
- **c** State what the number 6 in each isotope means.
- **d** Identify the number of protons, neutrons and electrons in each isotope.

2 Define the term 'relative isotopic abundance'.

3 Select the option that best identifies the reason for the distinctive yellow colour in a flame test of sodium nitrate.
- **A** The colour is due to sodium atoms losing an electron to form sodium ions.
- **B** The colour is due to electrons near the nucleus of the sodium atom absorbing energy.
- **C** The colour is due to sodium ions being converted to sodium atoms in the reducing flame.
- **D** The colour is due to excited electrons returning to lower energy levels and releasing energy.

4 An electron in a lithium atom gains enough energy to move from the $n = 1$ to the $n = 2$ shell. Select which option best describes the state of this lithium atom.
- **A** The lithium atom becomes a positively charged ion.
- **B** The lithium atom becomes a negatively charged ion.
- **C** The lithium atom becomes an atom in an excited state.
- **D** The lithium atom becomes an atom in the ground state.

5 What two measurements are obtained directly from the output of a mass spectrometer and can be used for analysing elements?

6 Explain the similarities and differences between emission and absorption spectra for the same metal.

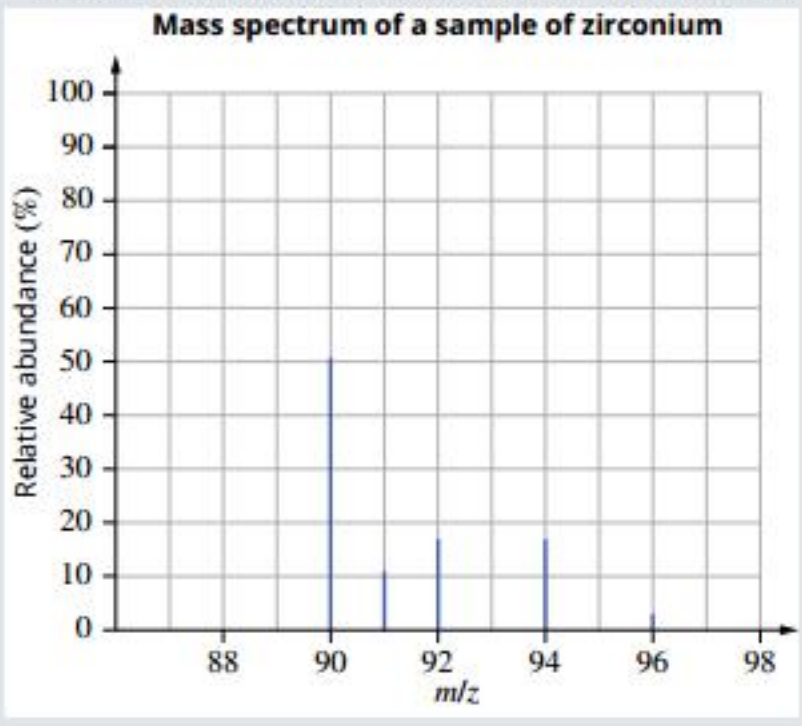
7 What is AAS and how can it be used to collect data? Explain how we can use this data.

8 Students recorded their observations when solutions of various compounds were sprayed into a Bunsen burner flame. Determine which one of the following observations is true.
- **A** Calcium chloride burns with a green flame.
- **B** Ammonium chloride burns with a yellow flame.
- **C** Potassium nitrate burns with a lilac flame.
- **D** Barium chloride burns with a colourless flame.

Apply

9 Determine the atomic number, mass number and symbol for the element that has 45 protons and 58 neutrons.

10 Explain how many isotopes are present in the mass spectrum of the sample of zirconium shown below.



11 Potassium chloride can be used as a replacement for table salt by people suffering from high blood pressure. While cooking, some potassium chloride was spilt in the flame of a gas stove.
- **a** Identify the colour of the flame that was observed.
- **b** Describe what would be observed if the potassium chloride contained some sodium chloride.

12 Explain why an emission spectrum contains a number of lines of different colours.

13 Explain how the absorption spectrum from a star is similar to a person's fingerprint.

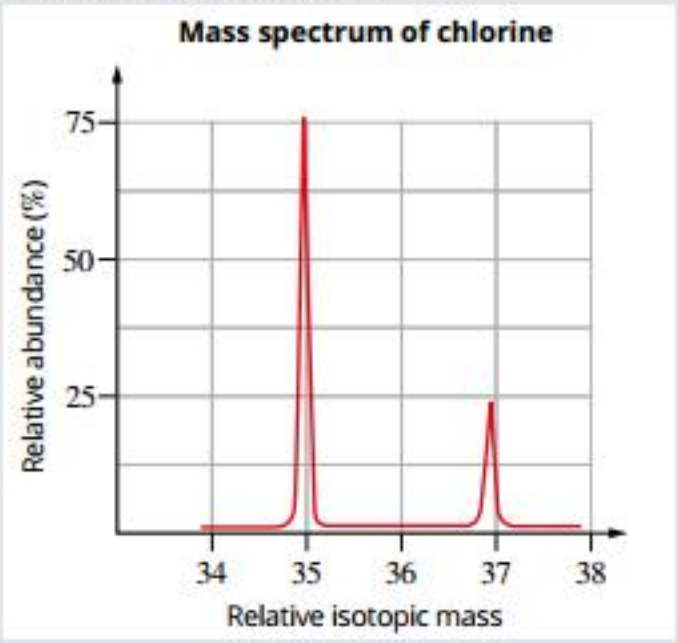
14 Explain how mass spectra are used to identify an element based on calculating its relative mass.

Analyse

15 For which of the situations below could you use atomic absorption spectrometry to obtain quantitative data? Explain your reasoning.

I mercury in a can of tuna
II salt in baby food
III carbon monoxide in natural gas
IV barium in an ore sample
V hydrocarbons in soil
VI aspirin in tablets

16 Consider the mass spectrum of chlorine shown below and the following statements.

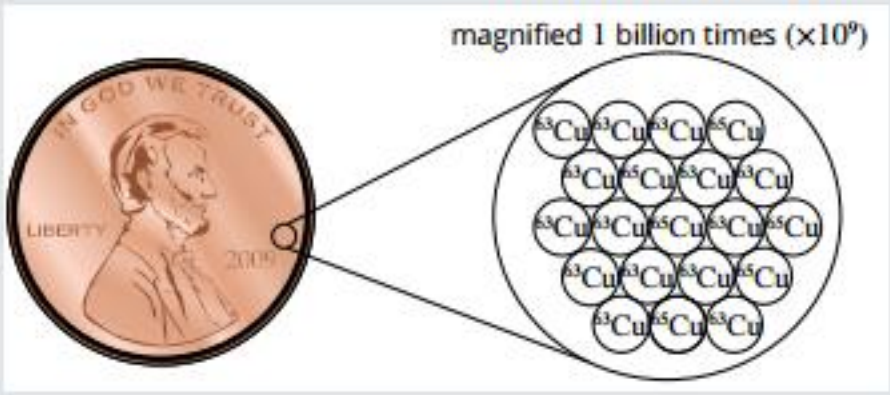


I The precise relative atomic mass of chlorine can be calculated by adding the two relative isotopic masses and dividing by 2.
II The lighter isotope is the less abundant.
III The isotopes have different masses because they have different numbers of protons.
IV The relative atomic mass of chlorine is based on the scale where carbon-12 has a mass of 12 exactly.
V The relative atomic mass of chlorine can be calculated by summing the products of the relative isotopic masses and their relative abundances, and dividing by 100.

In which of the following lists are all statements correct?

A II and III
B I and IV
C IV and V
D III, IV and V

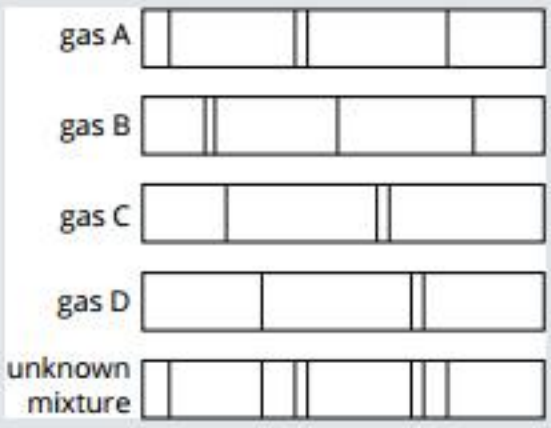
17 The elemental composition of a copper coin is shown in the diagram below. Calculate the relative atomic mass of copper using this information.



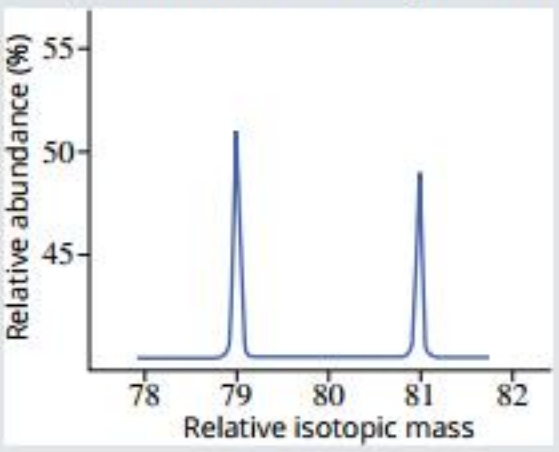
18 Barium and calcium are both group 2 elements. Explain why barium and calcium compounds produce different colours when they are held in a flame.

19 The standard on which all relative masses are based is the ^{12}C isotope, which is given a mass of 12 exactly. Why is the relative atomic mass of carbon 12.011?

20 Identify the two gases present in the mixture that produced the emission spectra shown in the diagram below.



21 The mass spectrum of bromine is given below.



a Using the values from this spectrum, complete the following table.

Isotopic mass	Relative abundance (%)

b Calculate the relative atomic mass of bromine.

22 Consider the following data about argon and potassium.

Element	Atomic number	Relative isotopic mass	Relative abundance (%)
argon	18	35.978	0.307
		37.974	0.060
		39.974	99.63
potassium	19	38.975	93.3
		39.976	0.011
		40.974	6.69

Which of the following statements is correct?

A The relative atomic mass of argon is 39.10; therefore, it is positioned before potassium in the periodic table.

B The relative atomic mass of potassium is 39.95; therefore, it is positioned after argon in the periodic table.

C Potassium has a lower percentage of heavier isotopes than argon, and is therefore positioned after argon in the periodic table.

D Argon has one less proton in the nucleus than potassium, and is therefore positioned before potassium in the periodic table.

23 The concentration of copper(II) ions in industrial wastewater was analysed by atomic absorption spectroscopy. The absorbance values from a series of standards and the wastewater are provided below.

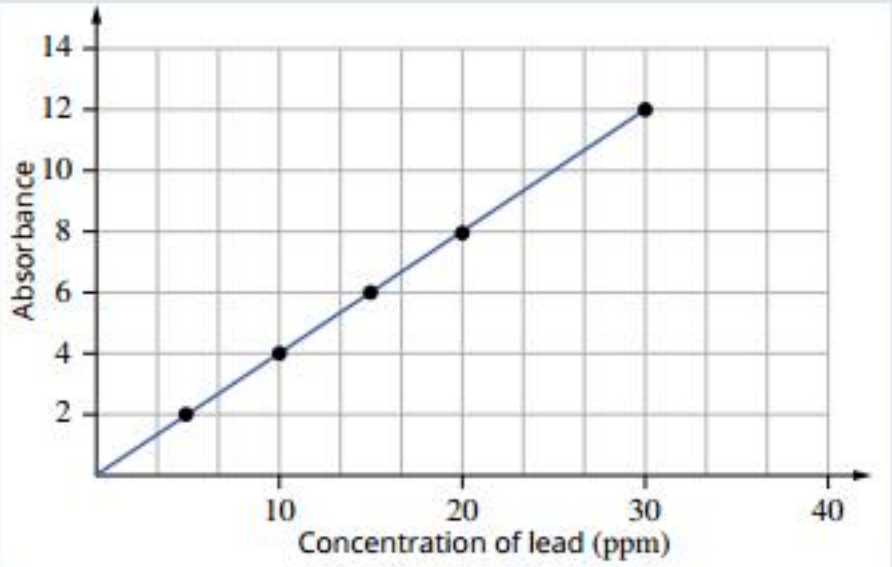
Concentration (mg L^{-1})	Absorbance
50	0.12
100	0.23
150	0.36
200	0.48
250	0.58
wastewater sample	0.40

Determine the concentration of copper(II) ions in the wastewater.

24 A batch of oysters was suspected of containing dangerous levels of lead. The following is an account of their analysis.

One of the oysters was removed from its shell and chopped finely in a food processor. A 1.50 g portion was heated on a hotplate with 10 mL of nitric acid. This mixture was filtered and then sprayed into the flame of an atomic absorption spectrometer. A hollow cathode lamp, which emitted light with a wavelength that is absorbed by lead atoms, was in place. The spectrometer measured an absorbance of 3.6 indicating that there was lead in the oyster.

To find the concentration of lead ions in the sample, the absorbance of different solutions containing known concentrations of lead ions was also measured. The results are graphed below.



The recommended limit of lead in oysters for human consumption is 2.5 ppm. Determine whether these oysters are fit to eat (1 ppm lead = 1 mg lead per kg oyster).

25 Element A occurs naturally in the environment. Scientists have found that a sample of this element contains 322 atoms of A-17, 569 atoms of A-18 and 2780 atoms of A-19. Calculate the relative atomic mass of the element A to 2 decimal places.

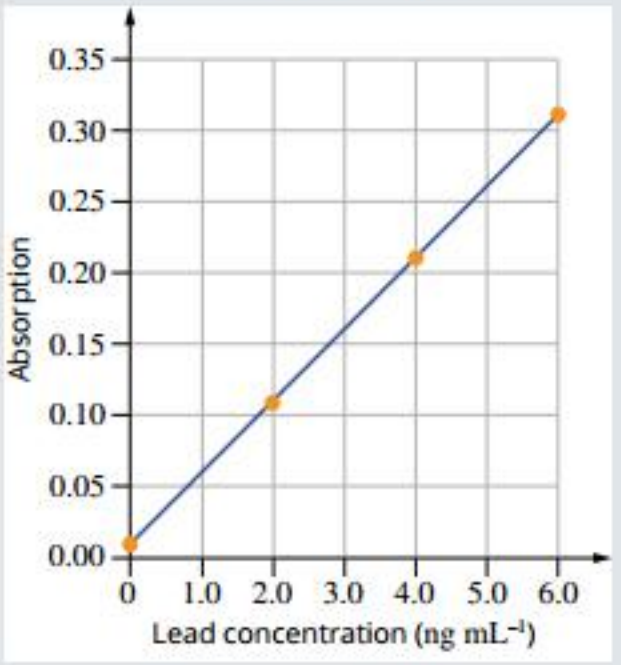
26 Use the data in Table 5.1.2 on page 82 to calculate the relative atomic mass of these elements.

a oxygen

b silver

c hydrogen

27 Lead exposure can cause permanent brain damage in infants and young children, even at very low levels. The amount of lead in infant milk formula can be measured by atomic absorption spectroscopy. A 2.5 g sample of milk powder was dissolved in 50 mL of distilled water. A very small volume of this solution was analysed and gave an absorbance of 0.130. Four standard solutions were analysed in the same way and the following calibration graph was obtained.



a Determine the concentration of lead ($ng\,mL^{-1}$) in the milk powder solution.

b Calculate the concentration of lead ($ng\,g^{-1}$) in the dried milk powder.

c Convert your answer to part **b** to ppm.

d Calculate the percentage by mass of lead in the milk powder.

e The zero standard, distilled water, gave an absorbance reading that was not zero. Suggest a reason for this.

28 The element lithium has two isotopes:

- ^{6}Li with a relative isotopic mass of 6.02
- ^{7}Li with a relative isotopic mass of 7.02.

The relative atomic mass of lithium is 6.94. Calculate the percentage abundance of the lighter isotope.

29 The relative atomic mass of europium is 151.96. The relative isotopic masses of the two isotopes of europium are 150.92 and 152.92. Calculate the relative abundances of the isotopes in naturally occurring europium.

Interpret

30 While sodium is an essential requirement in our diets, the amount of sodium consumed is often much higher than levels recommended by doctors. The sodium content of a sauce was determined using atomic absorption spectroscopy. A 25.00 mL sample of the sauce was diluted to 1.00 L with deionised water. Four standard solutions of NaCl were prepared and the absorbances of the four standard solutions and the diluted sauce solution were measured. The results are shown in the following table.

Concentration of Na^+ (aq) in $mg\,L^{-1}$	Absorbance
100	0.052
200	0.101
300	0.149
400	0.199
500	0.250
diluted sauce	0.184

a Create a calibration curve for Na^+.

b Use the calibration curve to determine the Na^+ concentration in the sauce.

c Determine the concentration of Na^+ in the original (undiluted) sauce in $g\,L^{-1}$.

d Identify what important assumption you must make to calculate the NaCl content of the sauce from the Na^+ concentration.

e If the daily recommended Na intake for a healthy adult is 2.5 g, calculate the amount of sauce a person would have to consume to exceed the recommended intake.

f Explain why the atomic absorption spectrometer will only measure the Na^+ concentration in your sample and not the concentration of other ions as well.

Data analysis

DATA SET 1

The information below applies to Questions 1–3.
The mass spectrum of chromium is shown in Figure 1.

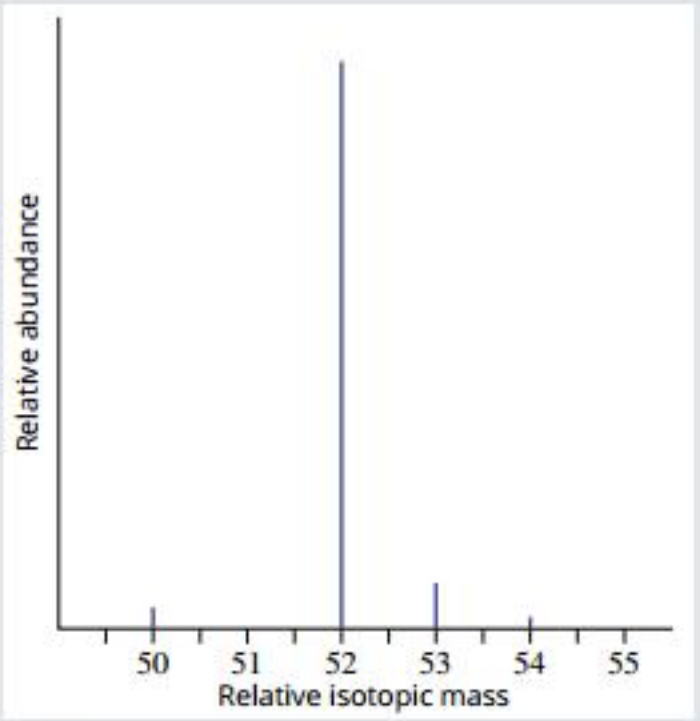


FIGURE 1 The mass spectrum of chromium. The relative abundances are given as peak heights and the relative isotopic masses have been simplified to 2 significant figures.

The accurate relative isotopic masses are given in Table 1.

TABLE 1 Relative isotopic mass of chromium isotopes

Isotope	Relative isotopic mass	Peak height	Percentage abundance
^{50}Cr	49.946		
^{52}Cr	51.941		
^{53}Cr	52.941		
^{54}Cr	53.939		

Question 1 (2 marks)

Measure the peak heights for each isotope and record the values in the table.

Question 2 (4 marks)

Calculate the percentage abundances of each chromium isotope and then record them in the table.

Question 3 (4 marks)

Use the percentage abundances calculated in Question **2** and the accurate isotopic masses to determine the relative atomic mass of chromium.

CHAPTER

06 Metals—bonding and properties

This chapter describes the properties and uses of metals and explains how the properties of metallic elements differ from those of non-metals. The properties of metals make them suitable for a wide range of everyday applications.

You will learn how chemists have been able to relate these properties to the structure of metals, and to explain their structure in terms of a metallic bonding model.

Metals can be modified by mixing them to make alloys. You will see how this modifies the structure of the metals and produces useful properties.

Syllabus subject matter

Topic 1 • Properties and structure of atoms

■ INTRODUCTION TO BONDING

- Explain that the ability of atoms to form chemical bonds is related to the arrangement of electrons in the atom and the stability of the valence electron shell. **6.1**
- Identify that the number of electrons lost, gained or shared is determined by the electron configuration of the atom. **6.2**
- Explain that chemical bonds are caused by electrostatic attractions that arise because of the sharing or transfer of electrons. **6.2**

Topic 2 • Properties and structure of materials

■ BONDING AND PROPERTIES

- Explain that the type of bonding within ionic, metallic and covalent substances determines their physical properties.* **6.2**
- Discriminate between ionic and metallic bonding. **6.2**
- Analyse data to determine the properties, structure and bonding of ionic, covalent and metallic compounds.* **6.2**

■ COMPOUNDS AND MIXTURES

- Identify that pure substances have distinct measurable properties (e.g. melting and boiling point, reactivity, strength, density) and mixtures have properties dependent on the identity and relative amounts of the substances that make them up. **6.3**

*The greyed-out section of this dot point is addressed explicitly in another chapter.

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6.1 Properties of metals

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the physical properties of metals
- recall the differences in properties between main group metals and transition metals.

Metals constitute more than 80% of the elements in the periodic table. Metals have been important to human beings since early times. The development of civilisation can be measured by the way humans have used metals. The Copper Age (5000–3000 BCE) was followed by the Bronze Age (3000–1000 BCE) and the Iron Age (from 1000 BCE).

Gold, silver and copper can be found on Earth in an almost pure form. These metals were employed by prehistoric humans to make ornaments, tools and weapons. As humans' knowledge of metallurgy (the science of modifying metals) developed, metals have played a central role in fields as diverse as construction, agriculture, art, medicine and transport.

In this module, you will examine the properties of metals and then learn about the bonding model that chemists have developed to explain these properties. This model has helped chemists and materials engineers to understand why metals behave the way they do and how metals can be modified to create useful new materials.

PROPERTIES AND USES OF METALS

The diverse properties of different metals make them suitable for many purposes. For example, titanium (Figure 6.1.1) is a very strong, relatively unreactive metal with a low density that is close to that of bone. Consequently, it is used in surgical implants that can last up to 20 years with little effect on the body. Titanium is also used in the aerospace industry, in art and architecture, and in sporting products such as golf clubs.

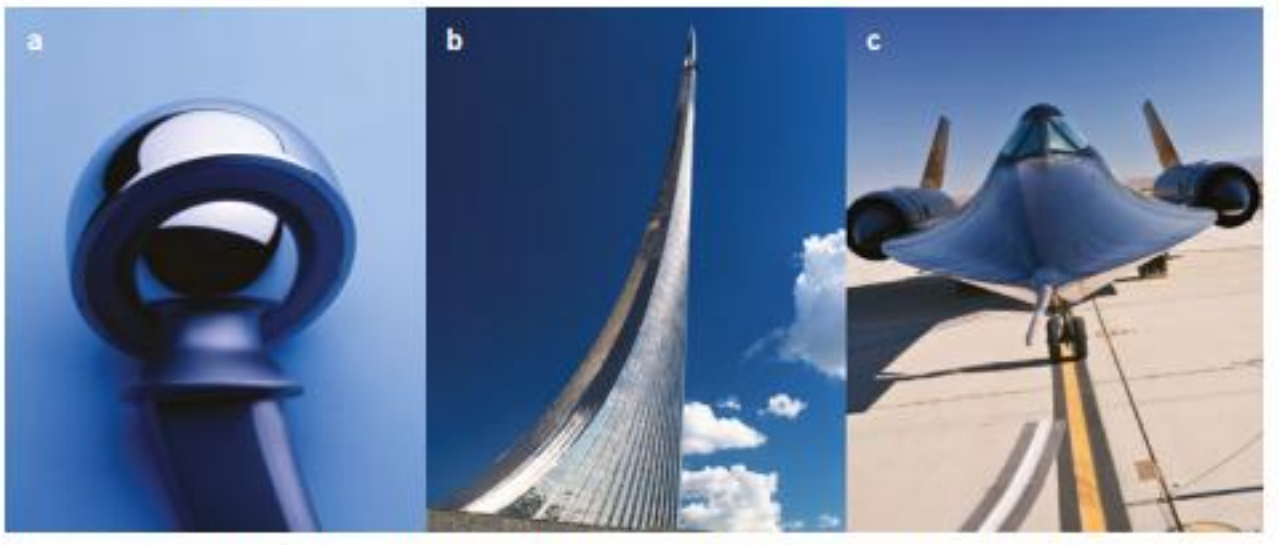


FIGURE 6.1.1 Titanium has many uses: (a) a replacement hip joint, (b) the spectacular curved space museum building in Moscow and (c) the SR-71 *Blackbird* reconnaissance aircraft. Although no longer manufactured, the SR-71 aircraft holds the world speed record (3530 km h^{-1}) for a manned aircraft that uses oxygen directly from the atmosphere.

Table 6.1.1 shows the uses of some metals.

TABLE 6.1.1 Properties and uses of some metals

Metal	Properties	Uses
iron	soft, malleable, magnetic, good thermal and electrical conductor, fairly reactive, readily forms alloys	can corrode and is usually converted to more stable steel, which is used in buildings and bridges, vehicles, machinery and appliances
aluminium	low density, relatively soft when pure, excellent thermal and electrical conductor, malleable and ductile, good reflector of heat and light, readily forms alloys	saucepans, frying pans, drink cans, cooking foil, food packaging, roofing, window frames, appliance trim, decorative furniture, electrical cables, aircraft and boat construction
titanium	very strong, high melting point, low density, low reactivity, readily forms alloys	medical devices within the body, wheelchairs, computer cases; lightweight alloys are used in high-temperature environments such as spacecraft and aircraft
gold	shiny gold appearance, excellent thermal and electrical conductor, unreactive, readily forms alloys	electrical connections, jewellery, monetary standard, dentistry

Table 6.1.2 gives the properties of some metals and non-metals.

Despite the range of properties, most metals:

- have relatively high boiling points (although they have a range of melting points)
- are good **conductors** of electricity
- are good conductors of heat
- generally have high **densities**.

TABLE 6.1.2 Properties of some metallic and non-metallic elements

Element	Melting point (°C)	Boiling point (°C)	Electrical conductivity ($MS\,m^{-1}$)*	Thermal conductivity ($J\,s^{-1}\,m^{-1}\,K^{-1}$)†	Density ($g\,mL^{-1}$)
Metals					
gold	1063	2970	45	310	19.3
iron	1540	3000	10.4	78	7.87
copper	1083	2567	59.6	385	8.96
mercury	–39	357	1	8.4	13.5
potassium	64	760	14	100	0.86
silver	961	2210	63	418	10.5
sodium	98	892	21	135	0.97
Non-metals					
carbon (diamond)	3550	‡	10^{-17}	–	3.51
oxygen	–219	183	–	0.026	1.15 (liquid)
sulfur	115	718	5×10^{-16}	0.205	1.92
fluorine	–220	–188	–	0.026	1.51 (liquid)
iodine	114	184	8×10^{-8}	0.45	4.9

*$MS\,m^{-1}$ = megasiemens per metre.

†Thermal conductivity measures the conductance of heat.

‡Diamond sublimes (changes straight from a solid to a gas) when heated.

FIGURE 6.1.2 This power transmission tower relies on the strength of steel for its structural integrity. The electrical cables are made from aluminium, utilising its tensile strength, ductility and electrical conductivity.

Not all metals have all of these properties. Mercury is a liquid at room temperature. It has an unusually low melting point. The group 1 elements (the **alkali metals**) have some properties that make them different to most other metals. They have low melting points, low densities, are all soft enough to be cut with a knife and they react vigorously with water to produce hydrogen gas. Both mercury and the group 1 elements exhibit most of the other properties of metals, and are therefore classified as metals. Being in group 1 at the left of the periodic table, alkali metals have the lowest ionisation energies and highest **metallic character**—they easily lose valence electrons.

The range of properties of different metals allows them to be used together to solve many engineering problems. The power transmission tower in Figure 6.1.2 is made from several metals to take advantage of their different properties.

Metals also generally have the following characteristics in common.

- They are **malleable**—they can be shaped by beating or rolling.
- They are **ductile**—they can be drawn into a wire.
- They are **lustrous**—they are reflective when freshly cut or polished.
- They are hard, with high **tensile strength** (resistance to breaking when pulled).
- They have low **electronegativities** and **ionisation energies**—their valence electrons are easy to remove.

Generally, metals are shaped for use in different applications by hammering, exploiting their malleability. Some metals, such as gold, copper and aluminium, are very malleable at room temperature. Other metals, such as iron, must be heated before they can be shaped.

TRANSITION METALS

Metals can be classified as main group metals or **transition metals**. Main group metals are found in groups 1, 2 and 13–16 of the periodic table. Between group 2 and group 13 is a block of elements known as the transition metals. These elements generally have unfilled *d* subshells and are often referred to as the *d*-block elements. They include metals such as iron and nickel that are used to build cities, bridges, cars and railway lines, and precious metals such as silver and gold that have ornamental and economic uses. Most transition metals are silver coloured and are similar in appearance, as shown in Figure 6.1.3.

FIGURE 6.1.3 The first row of transition metals

The transition metals are very important to Australian industry. All the metals in the first row of the *d* block are found in Australia and many are being mined today.

Iron is by far the most important metal to us. Nearly ten times more iron is mined than all other metals combined. Pure iron is relatively **brittle** (fractures easily) and corrodes easily. Iron is often combined with other transition metals and carbon (a non-metal) to produce **alloys** (homogenous mixtures) such as **steel**. Steel is a mixture of iron (~99%) and carbon (~1%) and has more desirable characteristics than pure iron. (Alloys are described in more detail in Module 6.3.)

FIGURE 6.1.4 Electrical cables used in domestic appliances. The copper wires inside the cables are coated with plastic insulation.

Copper is one of the few transition metals that is mainly used in its pure form. Its high electrical conductivity makes it especially useful for most of the millions of kilometres of electrical wires that enable the transmission of electric energy for heating, lighting, telephones, radio and television (Figure 6.1.4).

Transition metals are not only important for industry, but are also important for life. All the transition metals in the first row, except scandium and titanium, are essential for animal life. Your body relies on the presence of trace elements to carry out certain biochemical reactions. For example, chromium, which you get from meat and bread, assists in the production of energy from glucose.

Properties of transition metals

Compared to main group metals, transition metals have the following properties.

- They tend to be harder.
- They have higher densities.
- They have higher melting points.
- Some of them have strong magnetic properties.

The hardness, higher densities and higher melting points of transition metals are due to their atoms generally being smaller in size because of their greater effective nuclear charge. This allows them to pack together more tightly with stronger bonds. This decreased distance between atoms means that the **electrostatic attraction** between neighbouring atoms is greater and results in stronger bonding.

The high tensile strength of transition metals makes them suitable for use in the construction of buildings, cars, bridges and numerous other objects.

Transition metal compounds

Transition metal compounds display a wide range of different colours. They are extensively used as pigments in paints, and to colour glass, ceramics and enamel. In Figure 6.1.5, the colours used by the artists are created by the different transition metals present in the paint.

FIGURE 6.1.5 (a) *Homeward Laddie* (c. 1895) by Queensland artist Anthony Alder. (b) *Untitled* (2010) by artist Mavis Ngallametta, of the Wik and Kugu people of Aurukun, Far North Queensland. The pigments are made of ochre.

Ochre is a type of hard clay that contains iron oxides and hydroxides, which can be found naturally in many colours, including red, pink, white and yellow. Ground into a powder and mixed with liquids, ochre forms a paste that has been used for millennia by Aboriginal and Torres Strait Islander peoples in Australia for body decoration, cave painting, bark painting and other artwork.

The colours of many gemstones are also due to the presence of transition metals. For example, sapphires (Figure 6.1.6) contain traces of titanium and iron in a crystal of aluminium oxide.

The colours arise when electrons within the metal ions in the transition metal compounds absorb light of particular wavelengths and move to higher energy levels. Absorbance of light with some wavelengths and transmission of light with other wavelengths results in the compounds appearing coloured. In contrast, compounds of group 1 and group 2 metals are usually colourless.

FIGURE 6.1.6 Blue sapphires get their colour from impurities of titanium and iron.

6.1 Review

SUMMARY

- Metals have the following characteristic properties:
  - high boiling points
  - good conductors of electricity in solid and liquid states
  - malleable and ductile
  - high densities
  - good conductors of heat
  - lustrous
  - low electronegativities
  - low ionisation energies.
- The main differences between the properties of main group metals and transition metals are:
  - transition metals are harder
  - transition metals are more dense
  - transition metals have higher melting points
  - some transition metals have strong magnetic properties
  - transition metal compounds tend to be brightly coloured.

KEY QUESTIONS

Describe

1 List three properties common to most metals.

2 Explain the meaning of the term 'malleable' when referring to metals.

3 What are the main differences between the properties of main group metals and transition metals?

4 Name a metal that is a liquid at room temperature.

5 Which metal is mined the most in Australia? List three of its uses.

Apply

6 Explain the meaning of the term 'ductile' when referring to metals. How is this property different from malleability?

7 Classify the following metals as either main group metals or transition metals.

a K

b Al

c Ni

d Cu

e Pb

Analyse

8 Identify some physical and chemical properties *not* included in Table 6.1.2 on page 109 that you would need to consider before choosing between aluminium and iron for building a bridge.

9 Potassium is classed as a main group metal. Gold is a transition metal.

a Using the information provided in Table 6.1.2 on page 109, identify another metal that has similar physical properties to potassium.

b Using the information provided in Table 6.1.2 on page 109, identify another metal that has similar physical properties to gold.

c Identify the position of these four metals in the periodic table and give three differences between the two pairs of metals.

10 Explain the difference between metallic character and metallic properties.

11 A metallic element has the electron configuration $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$. Is the element a main group metal or a transition metal? Explain your reasoning.

12 Examine the information in Table 6.1.2 on page 109.

a Identify the properties of copper that make it a good choice for use in electrical wiring.

b If another metal was to be chosen for electrical wiring, explain what physical or chemical properties of the metal might influence your choice. Can you think of any other considerations that might influence your choice?

13 Give two reasons why the alkali metals (group 1) are not useful as structural metals.

14 Titanium is an important transition metal used in high-tech industries. Evaluate the physical and chemical properties of titanium that make this metal particularly useful for the aerospace industry.

6.2 Metallic bonding

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- recognise that the properties of metallic compounds can be explained by using the metallic bonding model
- understand the type of bonding within metallic substances.

In this module, you will learn how the properties of metals can be explained in terms of the arrangement of the particles in metals. You will also learn about the bonding model that chemists have developed to explain these properties. The metallic bonding model has helped chemists and materials engineers understand why metals behave as they do and how metals can be modified to create useful new materials.

RELATING STRUCTURE AND PROPERTIES

The properties of metals are listed in Table 6.2.1. Each of these properties gives some information about the structure and bonding of particles in metals.

TABLE 6.2.1 Properties of metals and resulting conclusions about metal structure and bonding

Property	What this tells us about structure
Metals are usually hard and tend to have high boiling points.	The forces between the particles must be strong.
Metals conduct electricity in both the solid and molten (liquid) states.	Metals have charged particles that are free to move in the presence of an electric field.
Metals are malleable and ductile.	The attractive forces between the particles must be stronger than the repulsive forces between the particles when the layers of particles are moved.
Metals generally have high densities.	The particles are closely packed in a metal.
Metals are good conductors of heat.	There must be a way of quickly transferring energy throughout a metal object.
Metals are lustrous or reflective.	Free electrons are present, so metals can reflect light and appear shiny.
Metals tend to react by losing electrons.	Electrons must be relatively easily removed from metal atoms.

Chemists have developed a model for the structure of metals to explain all the properties that have been mentioned so far. You can deduce from the information in Table 6.2.1 that the **metallic bonding model** must include:

- charged particles that are free to move and conduct electricity
- strong forces of attraction between particles throughout the metal structure
- some electrons that are relatively easily removed.

METALLIC BONDING MODEL

Electrons are the particles that enable metals to conduct electricity. They are able to move throughout the tightly packed arrangement of metal atoms (the **lattice**). Negatively charged electrons can be lost from the valence shell of metal atoms, forming positive ions (cations). As shown in Figure 6.2.1, the freed electrons **delocalise** (spread out) to form a 'sea' of electrons throughout the entire metal structure. The electrons are strongly attracted to the metal cations.

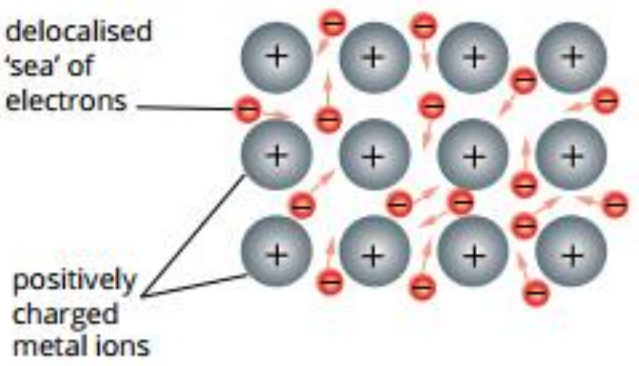


FIGURE 6.2.1 The metallic bonding model. Positive metal cations are surrounded by a mobile 'sea' of delocalised electrons. This diagram shows just one layer of metal ions.

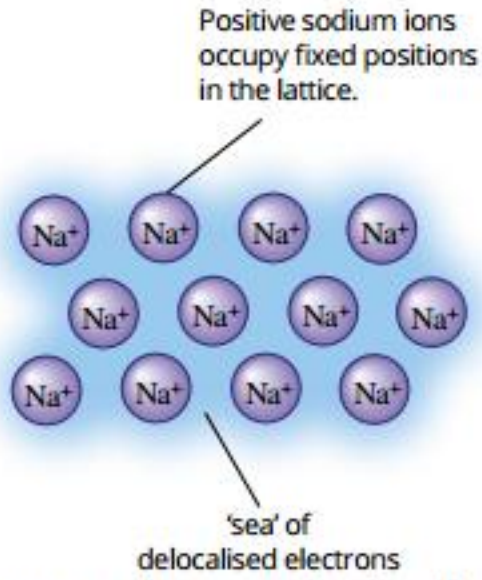


FIGURE 6.2.2 A representation of a sodium metal lattice. Each sodium atom loses its one valence electron. This electron is shared with all atoms in the lattice to form a 'sea' of delocalised electrons.

In the metallic bonding model, positive metal cations are surrounded by a 'sea' of delocalised electrons.

Chemists believe that in a solid sample of a metal:

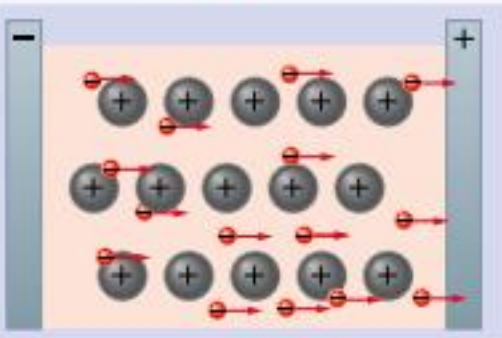
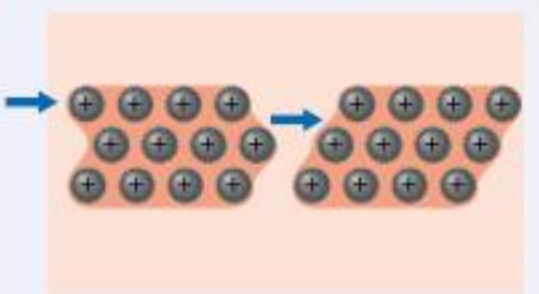
- Positive ions are arranged in a closely packed structure. This structure is described as a regular, three-dimensional network of positive ions (cations). The cations occupy fixed positions in the lattice.
- Negatively charged electrons move freely throughout the lattice. These electrons are called **delocalised electrons** because they belong to the lattice as a whole, rather than staying in the shell of a particular atom.
- The delocalised electrons come from the valence shells of the atoms. Inner-shell electrons are not free to move throughout the lattice and remain firmly bonded to individual cations.
- The positive cations are held in the lattice by the **electrostatic force** of attraction between these cations and the delocalised electrons. This attraction extends throughout the lattice and is called **metallic bonding**.

Together, these ideas make up the metallic bonding model. An example of how a metal, such as sodium, could be represented using this model is shown in Figure 6.2.2.

Relating the metallic bonding model to properties of metals

Table 6.2.2 shows how the metallic bonding model is consistent with key properties of metals, including relatively high boiling point, electrical conductivity, malleability and ductility.

TABLE 6.2.2 Physical properties of metals and explanations from the metallic bonding model

Property	Explanation	Example
Metals are hard and have relatively high boiling points.	Strong electrostatic forces of attraction between positive metal ions and the 'sea' of delocalised electrons hold the metallic lattice together.	
Metals are good conductors of electricity.	Delocalised electrons will move towards a positive terminal and away from a negative terminal in an electric circuit.	
Metals are malleable and ductile.	When a force causes metal ions to move past each other, layers of ions are still held together by the attractive forces from the delocalised electrons between them.	

Other properties of metals

Metals also have other properties that can be explained using the metallic bonding model.

- Metals generally have a high density. The cations in a metal lattice are closely packed. The density of a metal depends on the mass of the metal ions, their radius and the way in which they are packed in the lattice.
- Metals are good conductors of heat. When the delocalised electrons bump into each other and into the metal ions, they transfer energy to their neighbours. Heating a metal gives the ions and electrons more energy and they vibrate more rapidly. The electrons, being free to move, transmit this energy rapidly throughout the lattice.
- Metals are lustrous. Because of the presence of free electrons in the lattice, metals reflect light of all wavelengths and appear shiny.
- Metals tend to react by losing electrons. The delocalised electrons in metals may participate in reactions anywhere on the metal's surface. The **reactivity** of a metal depends on how easily electrons can be removed from its atoms and is related to the low ionisation energies of metals. This was covered in detail in Chapter 4.

Limitations of the model

Although this model of metallic bonding explains many properties of metals, some cannot be explained so simply. These include the:

- range of melting points, hardness and densities of different metals
- differences in electrical conductivities of different metals
- magnetic nature of some metals, such as cobalt, iron and nickel.

However, these are explained by a more complex model of metallic bonding, which is beyond the scope of this book.

Worked example 6.2.1

ELECTRON CONFIGURATION AND PROPERTIES OF ALUMINIUM

With reference to the electron configuration of aluminium, explain why solid aluminium can conduct electricity.	
Thinking	**Working**
Using the atomic number of the element, determine the electron configuration of its atoms. (You may need to refer to the periodic table at the end of the book.)	Al has an atomic number of 13. This means a neutral atom of aluminium has 13 electrons. The electron configuration is $1s^2 2s^2 2p^6 3s^2 3p^1$.
From the electron configuration, find how many valence shell electrons are lost to form cations that have a stable noble gas electron configuration. These electrons become delocalised.	Al has three electrons in its valence shell (the $3s^2 3p^1$ electrons). Al atoms will tend to lose these three valence electrons to form a cation with a charge of +3. The valence shell electrons become delocalised and form the 'sea' of delocalised electrons within the metal lattice.
A substance can conduct electricity if it contains free-moving charged particles.	If Al is part of an electric circuit, the delocalised electrons are able to move through the lattice towards the positive terminal of the circuit when an electric potential is applied.

➤ Try yourself 6.2.1

ELECTRON CONFIGURATION AND PROPERTIES OF MAGNESIUM

With reference to the electron configuration of magnesium, explain why solid magnesium can conduct electricity.

6.2 Review

SUMMARY

- Metallic bonding is the electrostatic force of attraction between a lattice of positive ions and delocalised valence electrons. The lattice of cations is surrounded by a 'sea' of delocalised electrons.
- The metallic bonding model can be used to explain the properties of metals, including their malleability, thermal conductivity, generally high melting point and electrical conductivity.

KEY QUESTIONS

Describe

1 **a** Describe what is meant by the following terms based on your understanding of the metallic bonding model.
- **i** delocalised electrons
- **ii** a lattice of cations
- **iii** metallic bonding

b Which electrons are delocalised in a metal?

2 Why is the bonding in metals described as 'electrostatic'?

3 Why are metals good conductors of electricity?

4 Using the metallic bonding model, explain why metals can be lustrous.

Apply

5 The properties of calcium mean that it is classed as a metal.
- **a** Draw a diagram to represent a calcium metal lattice.
- **b** Describe the forces that hold this lattice together.

6 Barium is an element in group 2 of the periodic table. It has a melting point of 850°C and conducts electricity in the solid state. Describe how the properties of barium can be explained in terms of its bonding and structure.

7 The electron configuration of magnesium is $1s^2 2s^2 2p^6 3s^2$. What will be the charge on the cations of magnesium in its metal lattice if it loses all its valence electrons?

8 Draw a diagram to show the movement of particles in a wire that is connected to the positive and negative terminals of a battery. Show and label the metal cations and electrons.

Analyse

9 Determine the charge of the cations formed from the following metals if they lose all their valence shell electrons.
- **a** Li
- **b** Mg
- **c** Ga
- **d** Ba

10 A very useful property of metals is that they are malleable.
- **a** Explain what specific part of the metallic bonding model enables metals to have this property.
- **b** Describe, with the aid of a diagram, what happens to a solid metal when a force is applied.

11 Determine why copper can conduct electricity, with reference to its electron configuration.

12 Graphite is a non-metallic form of carbon. It conducts electricity and can be lustrous. What can you deduce about the structure of graphite given that it shares some properties with metals?

6.3 Metallic mixtures—alloys

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- recognise that metals can be modified so that their physical and chemical properties can be altered
- compare the types and amounts of the substances that make up the modified metal to see what desirable properties can be obtained
- recognise that pure metals have distinct measurable properties (e.g. melting and boiling points, strength, density), whereas the properties of alloys depend on the identity and relative amounts of the substances that make them up.

The way in which a metal can be used is determined by its physical and chemical properties. Although some metals are valuable in their pure state, pure elements have distinct, fixed properties and most metals need to be modified to make them more useful.

Modified metals have a wide range of applications. Figure 6.3.1 shows two uses of modified metals. In each case, the properties of a metal have been improved by the process of alloying described in this module.

FIGURE 6.3.1 (a) Modified metals are used in aeroplanes, which need to be made from materials that are strong, durable and light. (b) The Oscar statuettes are made of britannium (a mixture of tin, copper and antimony) and then coated successively in layers of copper, nickel, silver and gold.

MAKING ALLOYS

Often, metals are mixed with small amounts of another substance, usually another metal or carbon. The substances are added to the molten metal and the mixture is then allowed to cool. The resultant solid is called an alloy.

By varying the composition of alloys, you can obtain materials with specific properties. Generally, an alloy is harder and melts at a lower temperature than the pure metal. This is because atoms of different sizes are now included in the metal lattice. As these atoms do not pack in the same way as the main metal, they will not allow the lattice to shift and bend in the same way. This disruption of the regular metallic lattice of the base metal by atoms of the added substance also accounts for the lowered melting point because it can weaken the metallic bonds between the atoms.

When other metals or carbon are added to melted metals, the substance that is produced is called an alloy. Alloys tend to have improved properties compared to the original metal, making them more useful in society.

Alloys of iron: steel

Currently, almost all of the iron mined around the world is used to make the alloy steel. The simplest steel is made by adding a small amount of carbon to iron to make carbon steel.

Carbon steel is a type of **interstitial alloy**. In interstitial alloys, a small proportion of an element with significantly smaller atoms is added to a metal. The added atoms sit in interstices (very small spaces) between metal cations in the metallic lattice, as shown in Figure 6.3.2.

Carbon steel is generally harder and less malleable than pure iron. Varying the amount of carbon in the mixture produces steels with different properties, as shown in Table 6.3.1. This allows the steel with the most suitable properties to be used in specific applications.

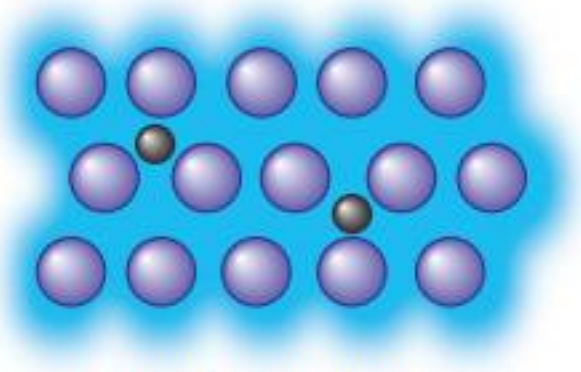


FIGURE 6.3.2 Steel is an interstitial alloy of iron and carbon. Note the relative sizes and position of the atoms in an interstitial alloy.

TABLE 6.3.1 A summary of the properties and uses of some different carbon steels

Type of carbon steel	Percentage of carbon	Properties	Typical use
low-carbon steel	less than 0.3%	strong, easily shaped	bridges, buildings, ships and vehicles
medium-carbon steel	0.3%–0.45%	increased hardness and tensile strength, decreased ductility	large machinery parts
high-carbon steel	0.45%–0.75%	very strong, more brittle	springs and high-strength wires
very high-carbon steel	up to 2.5%	hard, more brittle	cutting tools

Other elements can also be added in addition to carbon to make steels with improvements to different properties. Examples of some of these are listed in Table 6.3.2.

TABLE 6.3.2 Some elements that are alloyed with iron to make steels

Alloying element	General effects on properties	Typical use
manganese	increases strength and toughness	bicycle frames
chromium	increases hardness and tensile strength, resists corrosion	stainless steel for cutlery, kitchen sinks
nickel	increases toughness, tensile strength and hardness, resists corrosion	stainless steel
cobalt	improves magnetic properties, resists high temperatures	alnico magnets, jet propulsion engines

The steels in Table 6.3.2 are not considered to be interstitial alloys, as the added atoms are too big to fit into the spaces in the metallic lattice. The atoms of the added elements replace some of the iron cations and the mixture is called a **substitutional alloy** (Figure 6.3.3). In general, the metallic elements added to make substitutional alloys have similar chemical properties and form cations of a similar size to the main metal.

Stainless steel is a substitutional alloy of iron that usually contains nickel and chromium. The nickel and chromium atoms take the place of some of the iron atoms in the lattice. All the metal cations are attracted to the sea of electrons, so the lattice is still strongly bonded. However, because the different kinds of atoms are slightly different in size, the layers within the lattice cannot move as easily past each other. This makes the alloy harder and less malleable than pure iron.

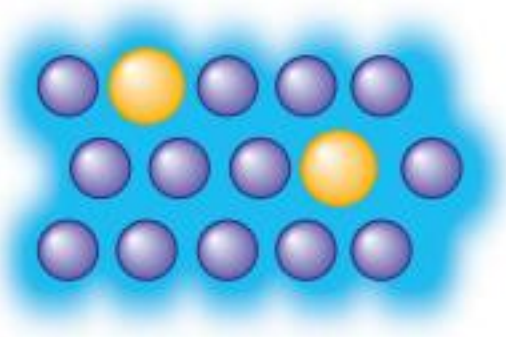


FIGURE 6.3.3 In a substitutional alloy, the atoms are relatively similar in size. Atoms of the alloying metal replace atoms of the original metal.

Common alloys

Many common materials are made of alloys to make the metal more suitable for a particular purpose. Metals are blended together to combine properties, such as strength, colour, reflectivity and chemical stability. The resulting alloy will have different properties from the individual elements. A number of examples of substitutional alloys are shown in Table 6.3.3.

TABLE 6.3.3 Substitutional alloys found in everyday objects

Alloy	Metals used	
Australian 20-cent coin	copper and nickel	
Australian $2 coin	copper, aluminium and nickel	
dental mercury amalgam	mercury and silver	
brass	copper and zinc	
bronze	copper and tin	

6.3 Review

SUMMARY

- Most metals can be modified to alter their properties and make them more useful.
- An alloy is a mixture of a metallic element with one or more other elements.
- Alloys are often harder and melt at a lower temperature than pure metals.
- Pure metals have distinct measurable properties, whereas the properties of alloys depend on the identity and relative amounts of the substances that they are made from.

KEY QUESTIONS

Describe

1 What is steel composed of?

2 State the difference between a substitutional alloy and an interstitial alloy.

3 Recall the alloys that make up an Australian 20-cent coin and high-carbon steel.

a List the elements present in each alloy.

b Draw a diagram to show how the atoms of these elements are arranged in each alloy.

Apply

4 Why are alloys described as having metallic lattices, even though they can be regarded as a type of mixture?

5 How can the properties of the element iron be modified when it is made into an alloy?

6 Explain why alloys tend to be harder and melt at a lower temperature than the pure metal from which they are made.

Analyse

7 A bicycle developer decides that manganese is too expensive for the frames he wishes to make. He looks at a range of metals as other options for the steel frame. For each metal listed below, determine the effects the addition of the metal to iron might have and whether these properties would be useful for the bike frame.

a chromium

b nickel

c cobalt

d lithium

e aluminium

8 For each of the following alloys, determine the alloy type (interstitial or substitutional). You may need to refer to Appendix D: Atomic and ionic radii of selected elements on page 519.

a copper/beryllium

b iron/chromium

c aluminium/magnesium

9 Determine which of the properties listed below match each of the alloys.

I high strength, light weight

II high strength, excellent electrical conductivity

III increased strength, increased resistance to corrosion

a copper/beryllium

b iron/chromium

c aluminium/magnesium

Chapter review

06

KEY TERMS

alkali metal
alloy
brittle
conductor
delocalise
delocalised electron
density
ductile
electronegativity
electrostatic attraction
electrostatic force
interstitial alloy
ionisation energy
lattice
lustrous
malleable
metallic bonding
metallic bonding model
metallic character
reactivity
steel
substitutional alloy
tensile strength
transition metal

KEY QUESTIONS

Describe

1 A ductile material:
- **A** can be rolled into thin sheets
- **B** can be drawn out into wires
- **C** is very flexible
- **D** has a high density

2 Metals can conduct electricity in the solid state. Metals conduct electricity because:
- **A** their atoms are closely packed
- **B** metal ions can move easily through the lattice
- **C** valence electrons can move easily throughout the lattice
- **D** particles are weakly bonded in the solid

3 Which one or more of the following metals would have similar properties to barium?
Ca, Cs, Cu, Pb, Mg, Zn, Sr, K

4 Use a diagram to help describe what is meant by the term 'metallic lattice'.

5 What is an alloy?

6 Carbon forms an alloy with iron called steel. The main advantage of the presence of carbon in the iron is:
- **A** decreased rate of corrosion
- **B** increased malleability and ability to be welded
- **C** increased electrical conductivity
- **D** increased tensile strength and hardness

7 Select the correct words in the paragraph below to complete the following description of metallic bonding.
Metallic bonding arises from a force that is *electrostatic/magnetic* and *attractive/repulsive*. The *electrons/protons* in a metal are *localised/delocalised* and are attracted to *negatively/positively* charged *anions/cations*. Metallic bonding explains many *physical/chemical* properties of metals, such as malleability.

Apply

8 The following table presents some properties of three substances.

	Melting point (°C)	Electrical conductivity of liquid	Electrical conductivity of solid
X	810	good	poor
Y	1083	good	good
Z	8.4	poor	poor

- **a** Which of the substances is likely to be a metal?
- **b** What feature of metallic bonding accounts for the melting point of the metal compared to those of the other substances?

9 Metals can be classified as main group metals or transition metals. Consider the following metallic elements:
Na, Sn, Au, Ca, Mg, Fe
- **a** Which of these metals are transition metals?
- **b** How do the properties of transition metals compare with those of main group metals?
- **c** Explain the source of the differences in properties of the two types of metals.

10 Describe the arrangement of particles in a metal wire and explain how they allow the wire to conduct electricity.

11 Use the metallic bonding model to explain each of the following observations.
- **a** Copper wire conducts electricity.
- **b** A metal spoon used to stir a boiling mixture becomes too hot to hold.
- **c** Iron has a high melting point, 1540°C.
- **d** Lead has a density of $11.4\,g\,mL^{-1}$, which is much higher than that of a non-metal such as sulfur.
- **e** Copper can be drawn out to form a wire.

Analyse

12 Alloys are modified metals. For each example, identify the metals used and suggest one property that is different from the original metals.
- **a** an Australian $2 coin
- **b** stainless steel
- **c** dental mercury amalgam

13 Referring to Table 6.1.2 on page 109, which property most clearly distinguishes metals from non-metals?

14 Metals have many uses in modern society.
- **a i** Identify one metal that is used in large quantities in Australia's building industry.
- **ii** List the properties that make this metal suitable for this use.
- **iii** Determine the properties of this metal that might limit its use in buildings.
- **b i** Identify one metal that is used in large quantities for electrical wiring.
- **ii** List the properties that make this metal suitable for use in wires.
- **c i** Identify two metals that are used in large quantities in the jewellery trade.
- **ii** List the properties that make them suitable for this use.

15 Write the electron configurations for the metal ions in lattices of the following metals if all valence electrons are delocalised.
- **a** K
- **b** Mg
- **c** Na

16 Apply your knowledge and understanding of the physical and chemical properties of metals to determine which is the most useful property of each of the following metals.
- **a** aluminium
- **b** copper
- **c** steel

Interpret

17 It has been shown using X-rays that metals have an ordered, crystalline structure in the solid state.
- **a** Deduce, using the metallic bonding model, why metals form crystals.
- **b** Research the problems that can be caused by this crystalline structure when metals are used for particular applications.

18 Some metals are found as elements in nature; others are found as compounds, combined with other elements such as oxygen and sulfur in ores. Australia has natural reserves of many metals and ores, with mining producing large quantities of metals, including aluminium, copper, gold, iron and silver.
- **a** Show the chemical symbol for each of these metals.
- **b** Determine in which period, group and block of the periodic table each of these metals is found.
- **c** Suggest why gold and sometimes silver are found in nature as elements rather than as compounds.
- **d** Identify which of these metals are transition metals.

19 Arsenic ($Z = 33$) is near phosphorus, a non-metal, and the metals tin and lead in the periodic table.

Describe three tests or observations that you could make on a sample of arsenic (with appropriate safety precautions) to determine if it is best classified as a metal or non-metal.

20 Some elements of importance to society are called metalloids. Use the internet or other sources to answer the following questions.
- **a** What is a metalloid?
- **b** Name three metalloids.
- **c** Describe how two of the metalloids are used in the manufacturing industry.

CHAPTER

07 Ionic compounds

Rocks, ceramics and molten lava belong to a group of substances called ionic compounds. They form the majority of the Earth's crust and, when dissolved, are key components of biological systems. At the end of this chapter, you will be able to explain the structure and properties of these compounds.

Ionic compounds are made by the chemical combination of metallic and non-metallic elements. You will see that their properties are a direct result of the bonding between particles in the compound. The writing of chemical formulas and the naming of ionic compounds are other skills that you will learn in this chapter.

Syllabus subject matter

Topic 1 • Properties and structure of atoms

INTRODUCTION TO BONDING

- Explain that the ability of atoms to form chemical bonds is related to the arrangement of electrons in the atom and the stability of the valence electron shell. **7.2**
- Identify that the number of electrons lost, gained or shared is determined by the electron configuration of the atom. **7.2**
- State that transitional elements can form more than one ion. **7.2**
- Explain that ions are atoms or groups of atoms that are electrically charged due to an imbalance in the number of electrons and protons. **7.2, 7.3**
- Explain that chemical bonds are caused by electrostatic attractions that arise because of the sharing or transfer of electrons. **7.2**
- Determine the formula and IUPAC name of ionic and molecular compounds. **7.3**
- Discriminate between the terms *empirical formula*, *molecular formula* and the *formula unit*. **7.3**

Topic 2 • Properties and structure of materials

BONDING AND PROPERTIES

- Describe the properties of ionic, covalent and metallic compounds, e.g. melting and boiling point, thermal and electrical conductivity, strength and hardness.* **7.1**
- Explain that the type of bonding within ionic, metallic and covalent substances determines their physical properties.* **7.1**
- Explain the properties of ionic compounds by modelling ionic bonding as ions arranged in a crystalline lattice structure with strong electrostatic forces of attraction between oppositely charged ions. **7.1**
- Discriminate between ionic and metallic bonding. **7.2**
- Analyse data to determine the properties, structure and bonding of ionic, covalent and metallic compounds.* **7.1**

*The greyed-out section of this dot point is addressed explicitly in another chapter.

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7.1 Structure and properties of ionic compounds

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- recognise that ionic substances have similar physical properties, including high melting points, hardness, brittleness, solubility and an ability to conduct electricity when liquid or in an aqueous solution but not as a solid
- understand that the formation of ionic compounds can involve the transfer of one or more electrons between metal and non-metal atoms
- understand that ionic compounds have a neutral charge and are composed of a crystal lattice made of metal cations and non-metal anions held together by strong electrostatic forces of attraction
- understand key properties of ionic substances—high melting points, hardness, brittleness, electrical conductivity and solubility
- relate the physical properties of ionic substances to the structure of the ionic lattice.

You will recall from Module 4.4 that when a metal and a non-metal combine, electrons are transferred from one atom to the other, producing charged ions and creating a strong electrostatic attraction in the form of an ionic bond. In this chapter, you will learn how the structure and bonding within these **ionic compounds** dictate their physical and chemical properties, and how we can predict that an ionic compound will form from the nature of the elements involved in the compound.

PROPERTIES OF IONIC COMPOUNDS

If you think about the characteristics of rocks such as gemstones (Figure 7.1.1), kitchen crockery and table salt, you will recognise that these materials, and therefore ionic compounds, have some properties in common. Table 7.1.1 on page 125 lists some common properties of ionic compounds that can be found in materials you might encounter in everyday life. Note that the compounds listed are simple ionic compounds, whereas rocks, ceramics and bricks contain more complex ionic compounds.

Gypsum (calcium sulfate) is an ionic compound used to manage the chemistry of garden and farm soils. Table salt (sodium chloride) is also an ionic compound—**aqueous** sodium chloride is a small but key component of blood plasma, and is found in sports drinks designed to replenish body fluids. In the human body, sodium ions are essential for the conduction of nerve impulses, contraction and relaxation of muscles and maintenance of the body's overall fluid balance.

From these properties, we can infer certain characteristics about the structure of ionic compounds, including the nature of the chemical bonding that exists. For example, in Table 7.1.2 on page 125, we can see how the properties of sodium chloride can be related to the nature of the particles that make up this compound and how these particles are arranged, including the relative strength of the chemical bonding.

The ionic bonding model explains the strong forces of attraction between particles, as well as the presence of mobile charged particles in the molten state and in an aqueous solution.

Aqueous means that a substance is dissolved in water and is denoted by the bracketed state symbol (aq) that appears next to an aqueous species in a chemical equation.

FIGURE 7.1.1 Many gemstones are made from ionic compounds.

TABLE 7.1.1 Properties of typical ionic compounds

Ionic compound	Melting point (°C)	Conductive as solid	Conductive as liquid	Conductive in aqueous solution (0.1 mol L^{-1})	Solubility in water at 25°C (g/100 g water)	Example of commercially available product containing the compound
copper(II) sulfate	decomposes 110	no	yes	yes	22	bluestone spray (used to kill pathogens on fruit)
sodium chloride	801	no	yes	yes	36	food salt
calcium carbonate	1339*	no	yes	–	0.0013	main component in marble
zinc oxide	1975	no	yes	–	insoluble	zinc sunscreen
sodium hydroxide	318	no	yes	yes	114	drain cleaner

*Melting point determined under pressure to prevent decomposition of compound

We can use the information in Table 7.1.1 to show that ionic compounds generally have the following properties:

- They have a high **melting point** and **boiling point**—they are solids at room temperature.
- They are hard but **brittle**, unlike metals—therefore, they are neither malleable nor ductile.
- They do not conduct electricity in the solid state.
- They are good conductors of electricity in the liquid or aqueous state.
- They vary from very soluble to insoluble in water.

TABLE 7.1.2 Properties of sodium chloride and the information this provides about its structure

Property of sodium chloride	What the properties tell us about the structure of sodium chloride and other ionic compounds
high melting point	The forces of attraction between particles are strong.
hard but brittle	The forces of attraction between particles are strong, but particles break apart when a force is applied.
conducts electricity in the molten state or in an aqueous solution	Free-moving charged particles are present.
does not conduct electricity in the solid state	Charged particles may be present, but they are not free-moving in the solid state.

THE IONIC BONDING MODEL

The properties described above are a result of the arrangement and interaction between charged particles in ionic compounds. When metallic and non-metallic atoms react to form ionic compounds, the following two steps occur.

1 Metal atoms lose electrons to non-metal atoms, and so become positively charged **metal ions** (called **cations**). There are more protons than electrons, and so a **charge imbalance** exists.

2 Non-metal atoms gain electrons from metal atoms, and so become negatively charged **non-metal ions** (called **anions**). There are more electrons than protons, and so a charge imbalance exists.

You will remember from Module 3.3 how electrons arrange themselves into shells around the nucleus. Atoms are most stable when their valence shell is full. This means that there are eight electrons in the valence shell of atoms from period 2 onwards (Chapter 4). An atom's ability to form a cation or anion depends on how many electrons it needs to gain or lose to achieve this stable arrangement.

$X \rightarrow X^+ + e^-$
where X represents a metal element.

$Y + e^- \rightarrow Y^-$
where Y represents a non-metal element.

Newly formed cations and anions then arrange themselves in the following way.

- Large numbers of cations and anions combine to form a **three-dimensional lattice**.
- The three-dimensional lattice is held together strongly by electrostatic forces of attraction between the oppositely charged ions. The force of **electrostatic attraction** holding the ions together is called **ionic bonding**.
- The attractive force between ions of opposite charge outweighs the repulsive force between ions of the same charge, so the lattice is held together strongly.

$X^+ + Y^- \rightarrow XY$

Electrostatic forces of attraction exist between positive and negative charges.

A neutral ionic compound is formed when these charged ions bond.

The formation of ionic compounds is described in more detail in Module 7.2.

The formula of sodium chloride

The **chemical formula** of sodium chloride is written as NaCl (Figure 7.1.2). However, it is important to note that in a solid sample of an ionic compound, such as sodium chloride, individual pairs of sodium ions and chloride ions do not exist. In other words, the solid is not made up of discrete NaCl molecules.

Instead, the solid is made up of a continuous lattice of alternating Na^+ and Cl^- ions. All sodium ions are an equal distance from six chloride ions and all chloride ions are an equal distance from six sodium ions. The chemical formula NaCl is therefore known as a **formula unit**, which shows that the overall ratio of sodium ions to chloride ions in the lattice is 1:1. Writing chemical formulas is described in Module 7.3.

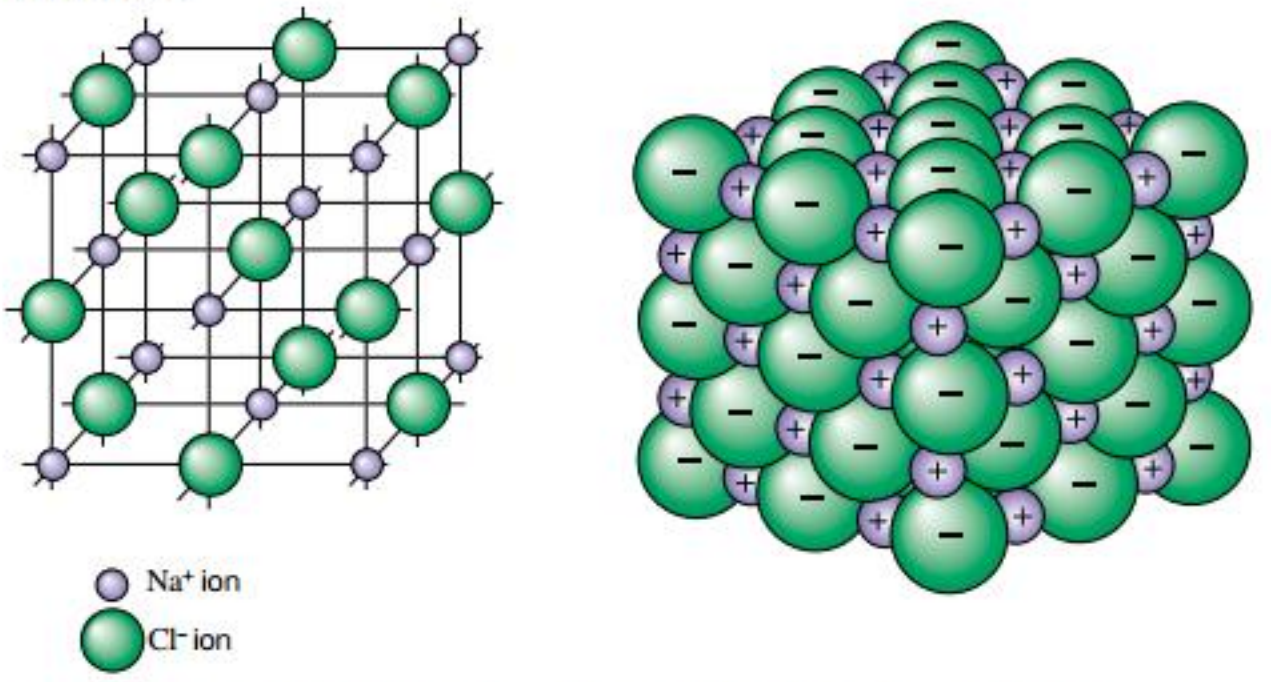


FIGURE 7.1.2 Two representations of a part of the crystal lattice of the ionic compound sodium chloride (NaCl). Forces of attraction (shown as lines in the first diagram) between oppositely charged ions result in strong bonding. Each positive sodium ion is surrounded by six negative chloride ions and each chloride ion is surrounded by six sodium ions.

USING THE IONIC BONDING MODEL TO EXPLAIN PROPERTIES

When comparing physical properties of ionic substances to other bonding types, you can see that ionic compounds have high melting points, as do metallic substances. Also, ionic substances have low electrical **conductivity** (in the solid state) in common with covalent substances. These and other properties can be related to the structure of ionic compounds. In Table 7.1.2, you saw that the properties of ionic compounds provided clues to their structure. Now, you will look in detail at those properties and how the ionic bonding model explains them.

High melting points

To melt an ionic solid such as sodium chloride, you must provide energy to allow the ions to break free of the ionic lattice and move apart from each other. When this energy is supplied (as heat), the increased kinetic energy of the ions disrupts the electrostatic attraction between them. The ions separate, causing the compound to change state from solid to liquid.

Sodium chloride has a high melting point (801°C). This indicates that a large amount of energy is needed to overcome the electrostatic attraction between oppositely charged ions and allow them to move freely. Therefore, the ionic bonds between the positive sodium ions and the negative chloride ions in the lattice must be strong. Generally, the stronger the bonds between ions, the higher the melting point.

The high melting point of ionic compounds is useful in some applications, such as in the bricks that line furnaces and kilns (Figure 7.1.3) and in the **ceramic** materials used to make brake discs for high-performance cars (Figure 7.1.4).

FIGURE 7.1.3 Bricks made from a mixture of ionic compounds that have high melting points are used to line furnaces and kilns.

FIGURE 7.1.4 Ceramic brake discs work more effectively than steel ones at high temperatures. A ceramic brake disc contains ionic compounds that have very high melting points and can withstand the heat produced by braking better than metals.

Hardness and brittleness

There are strong electrostatic forces of attraction between ions in an ionic compound, so a strong force is needed to disrupt the **crystal lattice**. Therefore, one of the properties of ionic compounds is that they are hard. This means that a sodium chloride crystal, for example, cannot be scratched easily.

The strength of house bricks, concrete bridges and cobbled streets can be attributed to the ionic bonding within their structures.

Some of the earliest tools used by humans were axes, spearheads and coarse needles used for weaving. Each application required a material that was hard and could be shaped. Certain types of rocks that are composed of ionic compounds served this purpose well. Figure 7.1.5 shows a stone axe head used by First Nations Australians more than 5000 years ago. This metamorphic basalt had been mined in a stone axe quarry at Lake Moondarra, on the traditional country of the Kalkadoon people, near Mt Isa. Stone axes from this quarry were traded widely around Australia and have been found in other locations up to 1000 kilometres from the quarry.

FIGURE 7.1.5 This axe head was found by archaeologists in a rock shelter in the Selwyn Range, north-western Queensland. It is at least 5000 years old.

The characteristic hardness of ionic compounds allows them to have other key roles.

- The calcium phosphate in bones makes them strong.
- Plasterboard contains calcium sulfate in the form of gypsum and is used for lining the walls and ceilings of houses.
- Granite, limestone and sandstone are used as building stone.

Although a salt crystal is hard, a strong force, such as a hammer blow, will shatter the crystal. Therefore, it is also brittle. This is because the layers of ions within the crystal lattice move relative to each other as a result of the force of the blow. During this movement, ions of like charge are shifted, so they are next to each other, as seen in Figure 7.1.6. The resulting repulsion between the similarly charged ions causes the crystal to shatter.

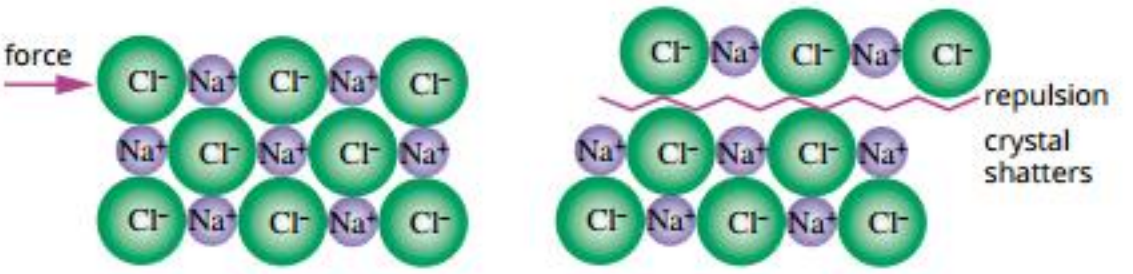


FIGURE 7.1.6 A lattice of an ionic compound shattering. Note that just before shattering, the Cl^- ions are next to other Cl^- ions and the Na^+ ions are also next to each other.

FIGURE 7.1.7 A porcelain coffee cup being smashed

Materials made from clay, such as kitchen crockery (Figure 7.1.7), ceramic tiles and bricks are hard, but they are also brittle. Porcelain is a type of chinaware made from a clay called kaolin. Clay is weathered rock and consists of a mixture of complex ionic compounds. The chemical formula for kaolin is $Al_2Si_2O_5(OH)_4$. The ions in kaolin are aluminium Al^{3+}, silicate $(Si_2O_5)^{2-}$ and hydroxide OH^-.

The brittleness of ionic compounds is very different to the properties of metals that we observed in the previous chapter. The malleability and ductility of metals were attributed to the sea of delocalised valence electrons, allowing relative freedom of movement of electrons between adjacent metal nuclei. The brittleness of ionic compounds suggests that the valence electrons of anions and cations remain fixed (i.e. localised) to their own nuclei. This makes sense since the formation of ions results in very stable valence shells where electrons are not readily shared or removed.

Electrical conductivity

In the solid form, ions in an ionic compound are held in the crystal lattice and are not free to move. Solid sodium chloride, for example, does not conduct electricity. Remember that for a substance to conduct electricity, it must contain charged particles that are free to move. The charged particles in an ionic compound are ions. Figure 7.1.8 on page 129 shows how the ions are arranged in an ionic compound in solid form.

The non-conducting property of solid ionic compounds is useful in **ceramic insulators**, which keep high-voltage powerlines insulated from electricity poles and electric fence wires (Figure 7.1.9 on page 129).

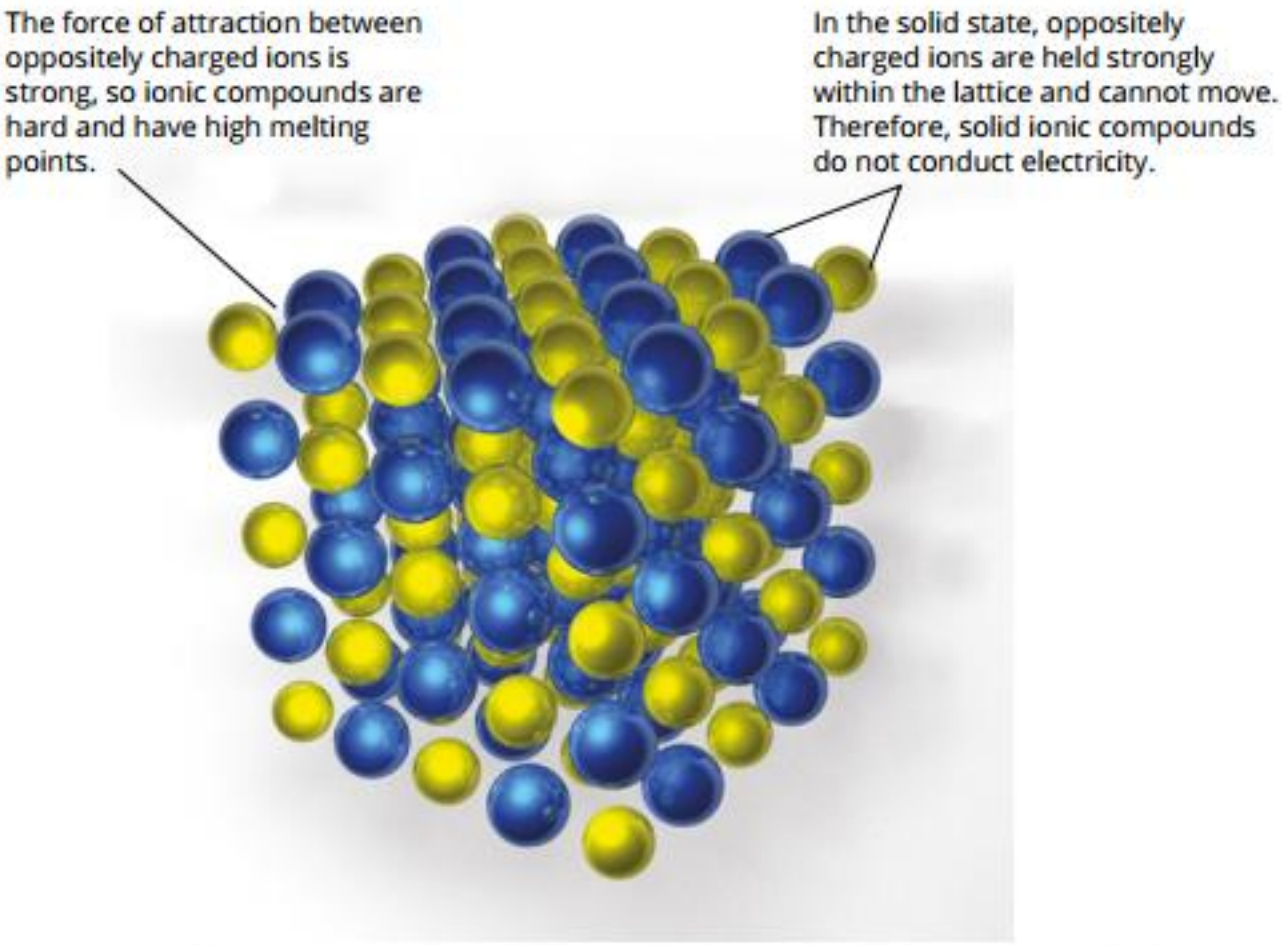

The force of attraction between oppositely charged ions is strong, so ionic compounds are hard and have high melting points.
In the solid state, oppositely charged ions are held strongly within the lattice and cannot move. Therefore, solid ionic compounds do not conduct electricity.

FIGURE 7.1.8 The arrangement of ions within a solid ionic compound. The strong crystal lattice structure explains its physical properties.

When solid ionic compounds **melt**, the ions become free to move, enabling the cations and anions in the molten (melted) compound to conduct electricity.

Similarly, when ionic compounds **dissolve** in water, ionic bonds in the lattice are broken, and the ions are separated and move freely in the aqueous solution.

When an electric **current** is applied to either a molten ionic compound or a solution of the compound in water, positive ions move towards the negatively charged **electrode** and negative ions move towards the positively charged electrode, resulting in an electric current as shown in Figure 7.1.10. A solution or molten substance that conducts electricity by means of the movement of ions in the liquid is called an **electrolyte**.

For an object to conduct electricity, it must contain charged particles that are free to move. Solid ionic compounds have a crystal lattice structure, so the particles are not free to move and they cannot conduct electricity. When molten (melted) or dissolved in water, the charged particles become free to move and conduct electricity.

Solubility

Some ionic compounds are **soluble** in water, whereas others are **insoluble**. When a soluble ionic compound is added to water, the ions are pulled away from the ionic lattice and mix with the water molecules to form a solution. If an insoluble compound is added to water, the ions remain bonded together in the ionic lattice and do not form a solution.

Whether an ionic compound is soluble or insoluble depends on the relative strength of the forces of attraction between the positive and negative ions in the lattice, and the water molecules and the ions—that is, the compound will be soluble if the forces between the water molecules and the ions in the lattice are strong enough to pull the ions out of the lattice. You will examine the solubility of ionic compounds in water in more detail in Chapter 13.

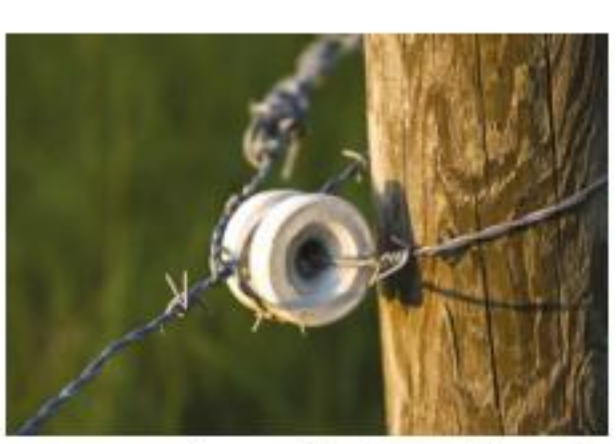


FIGURE 7.1.9 A ceramic insulator on the post of an electric fence

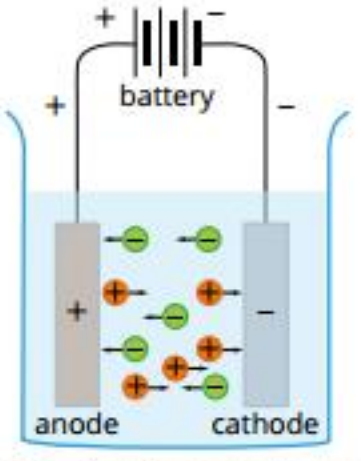


FIGURE 7.1.10 A molten ionic compound or a solution of the iconic compound will conduct an electric current.

7.1 Review

SUMMARY

- Ionic compounds form a crystal lattice made up of metal cations and non-metal anions.
- Each ion has a charge imbalance resulting from loss or gain of electrons.
- The three-dimensional lattice is held together strongly by electrostatic forces of attraction between the cations and anions. The electrostatic forces of attraction are called ionic bonding.
- In the case of sodium chloride, in order to maximise the forces of attraction, each sodium ion (Na^+) is surrounded by six chloride ions (Cl^-) and each chloride ion is surrounded by six sodium ions.
- Ionic compounds are hard and have high melting and boiling points. This is because of the strong forces of attraction between the positively and negatively charged ions in the ionic lattice.
- When an ionic compound is impacted by a strong force (e.g. hit by a hammer), the ions move within the lattice so that like-charged ions become close to one another and then repel, causing the lattice to be disrupted. This makes ionic compounds brittle.
- Ionic compounds do not conduct electricity in the solid state. Although the solid ionic lattice contains charged particles, the particles are not free to move.
- When ionic compounds are added to water or are in molten form, the charged particles are free to move, which means they can conduct electricity.
- In water, ionic compounds vary from very soluble to insoluble. The solubility depends on whether the forces between the water molecules and the ions in the lattice are strong enough to pull the ions out of the lattice.

KEY QUESTIONS

Describe

1 Select words from the following list to complete the sentences below. Words may be used more than once.

magnetic, lattice, non-metal, cations, valence, electrons, negatively, electrostatic, metal, positively, anions

Ionic compounds are formed when _____ atoms react with metal atoms. In this process _____ are transferred from metal atoms to _____ atoms, resulting in a full _____ shell for both atoms. Negatively charged non-metal ions called _____ and _____ charged metal ions called _____ are formed. The ions pack together in a three-dimensional _____ held strongly together by _____ attraction.

2 Use the ionic bonding model to explain why ionic compounds conduct electricity when molten but not as solids.

Apply

3 Identify the elements in the following list that could be present as positive ions in an ionic compound.

chlorine, oxygen, magnesium, copper, sodium, sulfur, argon, potassium, phosphorus, vanadium

4 Using the periodic table on page 10, determine whether each of the following is likely to be an ionic substance.

a magnesium bromide
b carbon dioxide
c sulfur trifluoride
d lithium oxide

5 Explain why ionic compounds have a high melting point.

6 **a** Describe what happens to ions in an ionic compound when the compound is hit with a heavy blow.
b Explain why this makes ionic compounds brittle.

Analyse

7 Use the data provided to explain why the following substance is an ionic compound.

It has a melting point of 308°C.
It does not conduct electricity at 250°C, but will conduct electricity at 350°C.

8 Tap water is safe for drinking and has dissolved minerals (most of which are dissolved ionic substances) used by the body. Deduce why these substances also make tap water an electrocution hazard.

bauxite, sphalerite, haematite

9 Ionic bonding is classified as a type of 'strong bonding'. Explain how three of the physical properties of ionic compounds provide evidence for this classification.

7.2 Formation of ionic compounds

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that metal atoms lose electrons to form positively charged ions (cations) and non-metal atoms gain electrons to form negatively charged ions (anions)
- determine the charge on an ion using its electron configuration and the octet rule
- understand that when an ionic compound is formed from cations and anions, the ions combine in proportions that produce a compound with an overall zero charge.

Some of the reactions that occur between metals and non-metals to form ionic compounds are very vigorous. The reaction between sodium and chlorine to form sodium chloride produces a lot of heat. You will remember from Chapter 4 that sodium is very reactive. At high temperatures, the production of sodium chloride from sodium metal and chlorine gas is explosive, producing a flame and large amounts of energy.

FORMING IONS

When metal atoms react with non-metal atoms to form an ionic compound the following changes occur.

- Metal atoms lose electrons to form positively charged **ions** (cations).
- Non-metal atoms gain electrons to form negatively charged ions (anions).

From Chapter 4, you will remember that most metals have low ionisation energies and low **electronegativities**. This means that non-metal atoms are usually more electronegative than metal atoms. In other words, non-metals have a stronger attraction for electrons than metals. In reactions that form ionic compounds, metal atoms transfer one or more valence electrons to non-metal atoms.

Most importantly, the ions that are formed usually have eight electrons in their **valence shell**—a stable electron configuration. The tendency for **elements** to react in such a way that their atoms have eight electrons in their **valence shell** is known as the **octet rule**. Noble gases (group 18) are elements that already have the most stable valence shell configuration. Therefore, another way of thinking about the octet rule is that atoms tend to gain or lose electrons to gain a stable electron configuration identical to that of the noble gas nearest to them on the periodic table. The formation of stable ions is a powerful driving force in reactions between metals and non-metals when they transfer electrons and produce ionic compounds.

When an atom loses electrons, it becomes a cation (positively charged) as the number of protons is greater than the number of electrons—there is a charge imbalance. The ion formed is written with a superscript + sign, indicating the charge. When there are two electrons lost, its charge is written as 2+ as a superscript.

$$X \rightarrow X^+ + e^-$$

When an atom gains electrons, it becomes an anion (negatively charged). This is written with a superscript – sign. If three electrons are gained, the charge is written as 3– as a superscript.

$$Y + e^- \rightarrow Y^-$$

In Chapter 4, you learnt that atoms of elements in group 1 of the periodic table have electron configurations with one electron in the valence shell. Therefore, elements in this group often form cations with a charge of 1+, as they readily lose this one valence electron. For example, potassium has a condensed electron configuration of [Ar]$4s^1$. It will readily lose the one electron in the valence shell to have an identical electron configuration to argon (the nearest noble gas) and a charge of 1+.

Metals in group 2 of the periodic table have electron configurations with two electrons in their valence shells. Therefore, they readily form ions with a charge of 2+ as they lose these two valence electrons.

Non-metals in group 16 have six electrons in their valence shells. Therefore, they readily gain two electrons to form anions with a charge of 2–. Group 17 non-metals have seven electrons in their valence shells. Therefore, they readily gain one electron to fill the valence shell and form anions with a charge of 1–. All ions have a full valence shell according to the octet rule. Therefore, the periodic table can be used as a quick reference point to identify the likely charge that ions will attain, so that we can begin forming ionic compounds and writing their chemical formulas. Figure 7.2.1 shows the charge on the most common ions formed relative to the group of the element.

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
H^+																	He
Li^+	Be^{2+}											B	C	N^{3-}	O^{2-}	F^-	Ne
Na^+	Mg^{2+}											Al^{3+}	Si	P^{3-}	S^{2-}	Cl^-	Ar
K^+	Ca^{2+}	Sc^{3+}	Ti^{3+} Ti^{4+}	V^{3+} V^{5+}	Cr^{3+} Cr^{2+}	Mn^{2+} Mn^{4+}	Fe^{2+} Fe^{3+}	Co^{2+} Co^{3+}	Ni^{2+} Ni^{3+}	Cu^{2+} Cu^+	Zn^{2+}	Ga^{3+}	Ge^{4+}	As^{3-}	Se^{2-}	Br^-	Kr
Rb^+	Sr^{2+}	Y^{3+}	Zr^{4+}	Nb^{5+} Nb^{3+}	Mo^{6+}	Tc^{7+}	Ru^{3+} Ru^{4+}	Rh^{3+}	Pd^{2+} Pd^{4+}	Ag^+	Cd^{2+}	In^{3+}	Sn^{4+} Sn^{2+}	Sb^{3+} Sb^{5+}	Te^{2-}	I^-	Xe
Cs^+	Ba^{2+}	La^{3+}	Hf^{4+}	Ta^{5+}	W^{6+}	Re^{7+}	Os^{4+}	Ir^{4+}	Pt^{4+} Pt^{2+}	Au^{3+} Au^+	Hg^{2+} Hg^+	Tl^+ Tl^{3+}	Pb^{2+} Pb^{4+}	Bi^{3+} Bi^{5+}	Po^{2+} Po^{4+}	At^-	Rn
Fr^+	Ra^{2+}	Ac^{3+}															

FIGURE 7.2.1 The periodic table showing the common ions formed by each element.

Transition metal ions

A **transition metal** forms one or more stable ions that have incompletely filled *d* orbitals. For example, copper can form Cu^+ ions with a charge of 1+, and Cu^{2+} ions with a charge of 2+. This is because the *s*, *p* and *d* subshells of these transition metals have similar energy levels. Two or more electron configurations of the metal ion have similar stability, although one is usually more common than the other.

Some other metals with ions that have variable charges are shown below:

- lead (Pb^{2+} and Pb^{4+})
- iron (Fe^{2+} and Fe^{3+})
- tin (Sn^{2+} and Sn^{4+}).

For compounds of transition metal ions, you need to specify the charge on the metal ion by writing a Roman numeral in brackets immediately after the metal in the name of the compound. For example:

- iron(II) chloride contains the Fe^{2+} ion
- iron(III) chloride contains the Fe^{3+} ion
- copper(I) sulfide contains the Cu^+ ion.

There are some transition metal ions that only form one ion, for example, zinc (Zn^{2+}), cadmium (Cd^{2+}) and silver (Ag^{+}). Because these transition metals do not form ions with different charges, a Roman numeral is not needed in their names, for example, zinc chloride $ZnCl_2$, cadmium sulfide CdS and silver bromide AgBr.

FORMING IONIC COMPOUNDS

When sodium (a metal) reacts with chlorine (a non-metal), an ionic compound is formed in two stages. Firstly, as seen in the previous module, each sodium atom loses one electron and each chlorine atom gains one electron.

After the electron is transferred:

- the sodium ions (Na^{+}) have the stable electron shell configuration of $[He]2s^22p^6$ (the same as its nearest noble gas, neon)
- the chloride ions (Cl^{-}) have the stable electron shell configuration of $[Ne]3s^23p^6$ (the same as its nearest noble gas, argon).

Figure 7.2.2 illustrates how, when sodium reacts with chlorine, an electron is lost by each sodium atom and gained by each chlorine atom. A diagram of this type is called an **electron transfer diagram**.

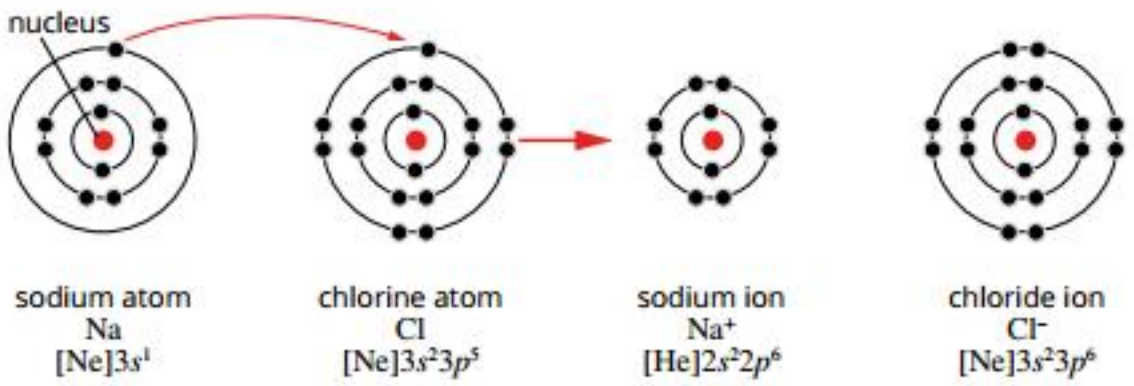


FIGURE 7.2.2 Electron transfer diagram showing the formation of sodium and chloride ions

In the second stage, the strong electrostatic attraction between Na^{+} and Cl^{-} draws the two ions together and forms an ionic bond as shown in the equation below. A neutral ionic compound containing charged particles is formed.

$$Na^{+} + Cl^{-} \rightarrow NaCl$$

When you write the formula of an ionic compound, you should write the **empirical formula**, the lowest whole number ratio of the atoms in the compound. This is because there are many millions of ions in an ionic crystal, so the most useful information is the ratio in which the ions combine. Ionic compounds do not exist as molecules, so this formula is referred to as a formula unit, the lowest ratio that produces a neutral electric charge, rather than a **molecular formula**, the actual number and type of atoms that would be present in a molecule. You will learn about molecular formulas in Chapter 8.

Let us look at the formation of two other ionic compounds, lithium oxide and magnesium chloride. The reaction between lithium and oxygen atoms is illustrated in Figure 7.2.3 on page 134. In this reaction, an oxygen atom needs to gain two electrons to have eight electrons in its valence shell and form a stable ion. Lithium has a single electron in its valence shell and loses one electron. To allow this to happen, one oxygen atom will react with two lithium atoms, taking one electron from each atom to produce a compound with an overall zero charge.

After the reaction, there are just two electrons in what is now the valence shell of the Li^{+} ion, which is the same as the electron configuration of a helium atom ($1s^2$). The oxygen ion has the same electron configuration as neon ($[He]2s^22p^6$).

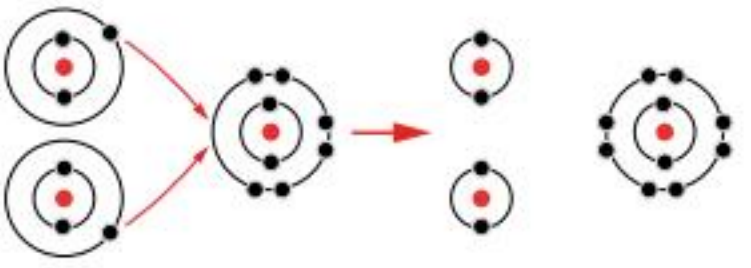
$$2Li^{+} + O^{2-} \rightarrow Li_2O$$

The strong electrostatic attraction between the two Li^{+} ions and one O^{2-} ion forms the ionic bond.

Ionic compound formation

Stage one $X + Y \rightarrow X^{+} + Y^{-}$

Stage two $X^{+} + Y^{-} \rightarrow XY$



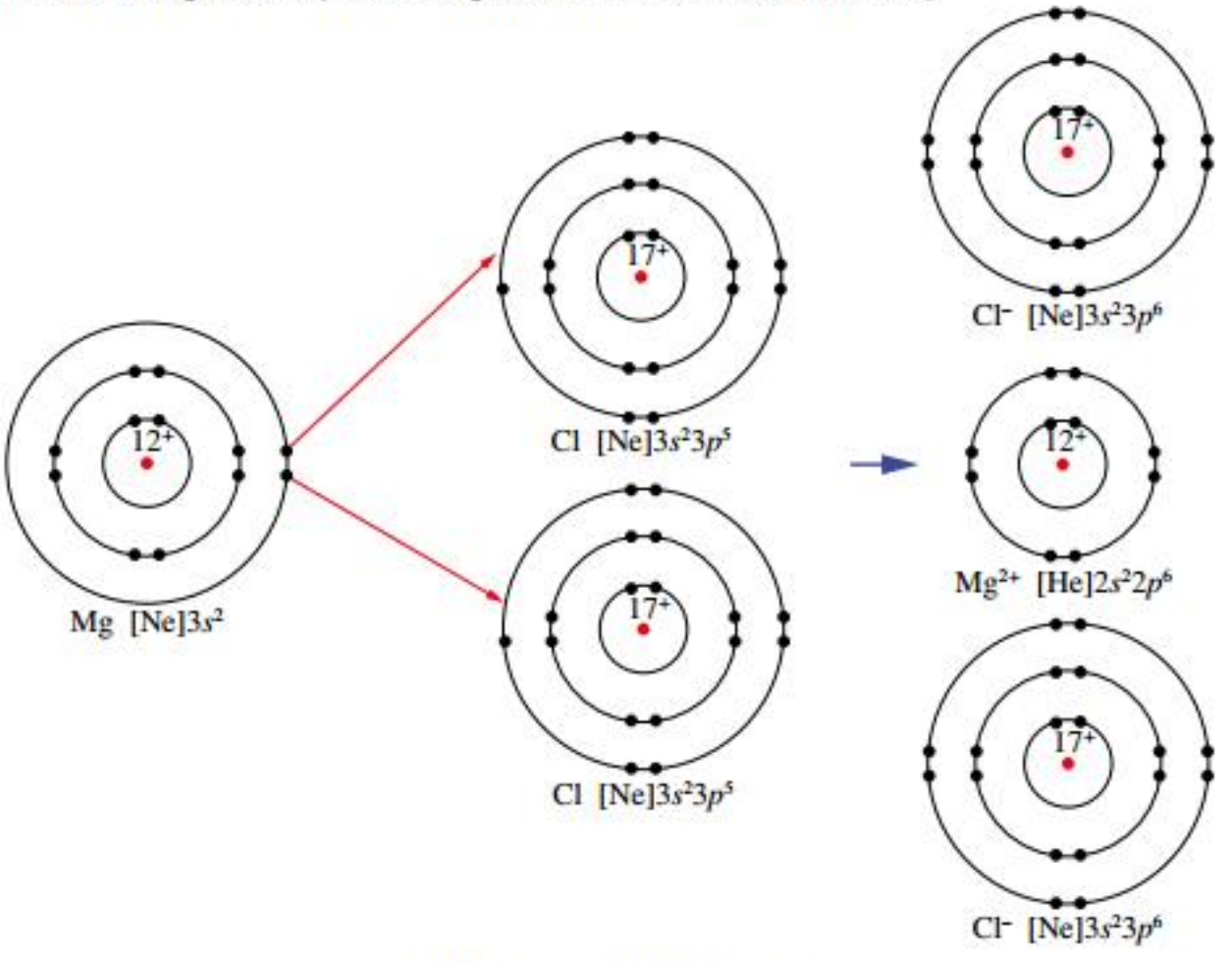
$$2Li + O \rightarrow 2Li^+ + O^{2-}$$
$$2Li^+ + O^{2-} \rightarrow Li_2O$$

FIGURE 7.2.3 Electron transfer diagram and chemical equation showing the formation of lithium oxide when lithium and oxygen react in a 2:1 ratio

The lithium symbol has a 2 as a subscript to show that two lithium ions are present in the compound. (This is explained further in Module 7.3.)

Figure 7.2.4 shows the electron transfer diagram and chemical equation for the reaction of magnesium with chlorine. Magnesium atoms have an electron configuration of [Ne]$3s^2$, so each magnesium atom will readily lose its two valence electrons. Magnesium ions (Mg^{2+}) are formed with the electron configuration of the nearest noble gas, neon ([He]$2s^22p^6$). Each chlorine atom has an electron configuration of [Ne]$3s^23p^5$, so each will gain one valence electron. A chloride ion (Cl^-) has the electron configuration of the noble gas argon ([Ne]$3s^23p^6$). Because magnesium readily donates two electrons, magnesium reacts in a 1:2 ratio, each chlorine atom taking one electron from magnesium to produce a compound with an overall zero charge.

The subscript 2 next to chlorine in the chemical formula shows the number of chloride ions present. (This is explained further in Module 7.3.)



$$Mg + 2Cl \rightarrow Mg^{2+} + 2Cl^-$$
$$Mg^{2+} + 2Cl^- \rightarrow MgCl_2$$

FIGURE 7.2.4 Electron transfer diagram and chemical equations showing the formation of magnesium chloride when magnesium and chlorine react in a 1:2 ratio.

You will learn how to write simple and more complex chemical formulas for ionic compounds in Module 7.3.

In an ionic compound, the total number of positive charges on the metal ions must equal the total number of negative charges on the non-metal ions.

Worked example 7.2.1

WRITING EQUATIONS FOR FORMATION OF AN IONIC COMPOUND

Develop an equation for the reaction between sodium and nitrogen atoms to form sodium nitride. Show the electron configurations for each element before and after the reaction and the chemical equation for the combination of the ions.	
Thinking	**Working**
Write the symbol and electron configuration of the metal atom.	Na ($[Ne]3s^1$)
How many electrons will the metal atom lose from its valence shell when it reacts?	1
Write the symbol and electron configuration of the metal ion that is formed.	Na^+ ($[He]2s^22p^6$)
Write the symbol and electron configuration of the non-metal atom.	N ($[He]2s^22p^3$)
How many electrons will the non-metal atom gain to fill its valence shell when it reacts?	3
Write the symbol and electron configuration of the non-metal ion that is formed.	N^{3-} ($[He]2s^22p^6$)
Calculate the lowest common multiple of the two numbers in the charges of the ions.	3
Calculate how many positive ions are needed to equal the lowest common multiple.	three Na^+ ions
Calculate how many negative ions are needed to equal the lowest common multiple.	one N^{3-} ion
Use the answers from the previous two steps to write the formula for the ionic compound using subscripts to show the number of ions. Write the symbol of the positive ion first. (Note that 1 is not written as a subscript.)	Na_3N
Write the chemical equation for the combination of sodium and nitrogen.	$3Na$ ($[Ne]3s^1$) + N ($[He]2s^22p^3$) → $3Na^+$ ($[He]2s^22p^6$) + N^{3-} ($[He]2s^22p^6$) $3Na^+ + N^{3-} \rightarrow Na_3N$

➤ Try yourself 7.2.1

WRITING EQUATIONS FOR FORMATION OF AN IONIC COMPOUND

Develop an equation for the reaction between calcium and phosphorus atoms to form calcium phosphide. Show the electron configurations for each element before and after the reaction and the chemical equation for the combination of the ions.

7.2 Review

SUMMARY

- During the formation of ionic compounds, an imbalance in the numbers of electrons and protons gives atoms a negative or positive charge.
- Metal atoms lose electrons to form positively charged ions (cations).
- Non-metal atoms gain electrons to form negatively charged ions (anions).
- The ions present in an ionic compound have a stable electron configuration identical to that of the noble gas nearest to them on the periodic table (the octet rule).
- For transition metals (and several other metals) that form ions with different charges, the charge on the ion is shown by placing a Roman numeral after the name of the metal.
- When an ionic compound is formed from cations and anions, the ions combine in proportions that produce a compound with an overall zero charge (refer to Module 7.3).

KEY QUESTIONS

Describe

1 Write the electron configuration of each of the following ions.

a K^+

b F^-

c Mg^{2+}

d Al^{3+}

2 State the charge on the transition elements that are represented as follows.

a iron(II)

b vanadium(III)

c copper(I)

Apply

3 Complete the table by writing the electron configuration of the element, whether electrons are lost or gained when an ion is formed, how many electrons are lost or gained, the number of protons and electrons in the ion, and the charge on the ion.

4 Explain why an ionic compound is formed when a metal reacts with a non-metal (rather than a metal with a metal, or a non-metal with a non-metal).

5 Use an electron transfer diagram to show the formation of ions when electrons are transferred between magnesium and fluorine.

6 Use the octet rule and refer to noble gas electron configurations to explain why group 2 metals of the periodic table are likely to form cations with a charge of 2+.

7 Determine the number of electrons lost or gained by copper when forming cations of 1+ and 2+ charges. Explain why copper forms two cations.

Analyse

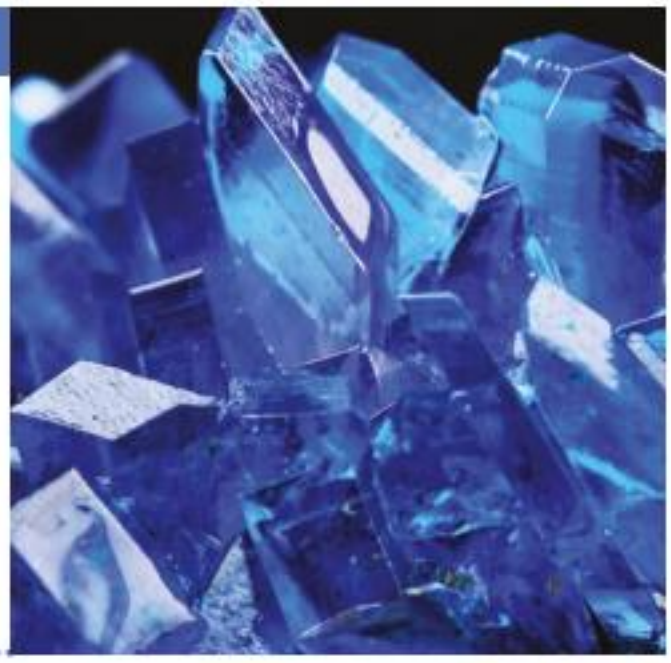
8 Consider the electron transfer diagram in Figure 7.2.4 on page 134 and explain why magnesium and chlorine react in a 1:2 ratio.

	Electron configuration	Electrons lost or gained?	How many electrons lost or gained?	Number of protons in the ion	Number of electrons in the ion	Charge on the ion
sodium						
calcium						
chlorine						
nitrogen						
oxygen						

7.3 Chemical formulas of ionic compounds

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- write formulas for ionic substances by determining the number of each ion in the formula unit based on the charge on the ion and the overall neutrality of the compound
- use rules to write formulas using symbols and subscripts
- use the chemical formula to determine the name of the compound
- understand that ions can be composed of more than one atom; these are called polyatomic ions
- use brackets to surround the polyatomic ion in a chemical formula when more than one polyatomic ion is required to make a neutral ionic compound; a subscript after the bracket indicates the number of polyatomic ions required in the formula.



You have seen that ionic compounds contain oppositely charged ions that are arranged in three-dimensional lattices. The charges on these ions arise from the transfer of electrons between atoms. An ionic crystal may contain billions of these ions in an immense three-dimensional lattice, so an empirical formula is used to describe the simplest ratio of ions in a neutral formula unit of the ionic compound.

WRITING THE FORMULA OF AN IONIC COMPOUND

Ionic compounds are electrically neutral because they are composed of positively and negatively charged ions formed by the initial transfer of electrons between metals and non-metals, followed by the combining of the ions into a compound. This means that the total number of positive charges on the metal ions must equal the total number of negative charges on the non-metal ions. This principle will guide you when trying to work out the formula of an ionic compound.

An example of this is the formula of the ionic compound magnesium chloride.

- A magnesium ion (Mg^{2+}) has a 2+ charge.
- A chloride ion (Cl^-) has a 1– charge.

Therefore, in a crystal of magnesium chloride, two chloride ions are needed to provide two negative charges so that they balance the 2+ charge on every magnesium ion. Therefore, the ratio of magnesium ions to chloride ions in the crystal is 1:2 and the formula of magnesium chloride is $MgCl_2$. The electron transfer diagram of this reaction is shown in Figure 7.2.4 on page 134.

Figure 7.3.1 on page 138 illustrates how formulas for some other ionic compounds can be determined. Tables 7.3.1 and 7.3.2 on page 138 list some of the more common positively and negatively charged ions. You may use these tables when you are writing formulas for ionic compounds. Remember that an ionic substance contains millions of ions, depending on the size of the crystal. Therefore, the ionic formula is known as a formula unit, which indicates the simplest whole number ratio of ions that make up the lattice.

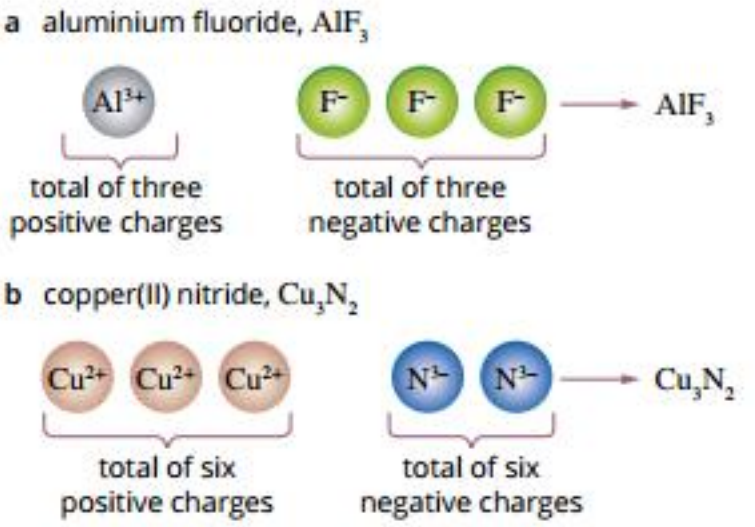


FIGURE 7.3.1 How to deduce chemical formulas from the charges on ions

In Module 7.2, you learnt that transition metals are able to form more than one ion. As seen in Table 7.3.1, the charge of the ion of a transition metal is taken from the Roman numeral that is in brackets after the name of the ion.

TABLE 7.3.1 Names and formulas of some common cations

Charge			
1+	2+	3+	4+
caesium, Cs^+ copper(I), Cu^+ gold(I), Au^+ lithium, Li^+ potassium, K^+ rubidium, Rb^+ silver, Ag^+ sodium, Na^+	barium, Ba^{2+} cadmium, Cd^{2+} calcium, Ca^{2+} cobalt(II), Co^{2+} copper(II), Cu^{2+} iron(II), Fe^{2+} lead(II), Pb^{2+} magnesium, Mg^{2+} manganese(II), Mn^{2+} mercury(II), Hg^{2+} nickel (II), Ni^{2+} strontium, Sr^{2+} tin(II), Sn^{2+} zinc, Zn^{2+}	aluminium, Al^{3+} chromium(III), Cr^{3+} gold(III), Au^{3+} iron(III), Fe^{3+}	lead(IV), Pb^{4+} tin(IV), Sn^{4+}

TABLE 7.3.2 Names and formulas of some common monatomic (single atom) anions

Charge		
1–	2–	3–
bromide, Br^- chloride, Cl^- fluoride, F^- iodide, I^-	oxide, O^{2-} sulfide, S^{2-}	nitride, N^{3-}

Rules for writing chemical formulas

Here are some rules to follow when you are writing chemical formulas. These rules are illustrated in Figure 7.3.2 on page 139.

- Write the symbol for the positively charged ion first.
- Use subscripts to indicate the number of each ion in the formula. Use the lowest common multiple of the two numbers in the charges of the ions to determine how many of each ion should be present. Write the subscripts after the ion they refer to.
- If there is just one ion present in the formula, omit the subscript '1'.
- Do not include the charges on the ions in the balanced formula.

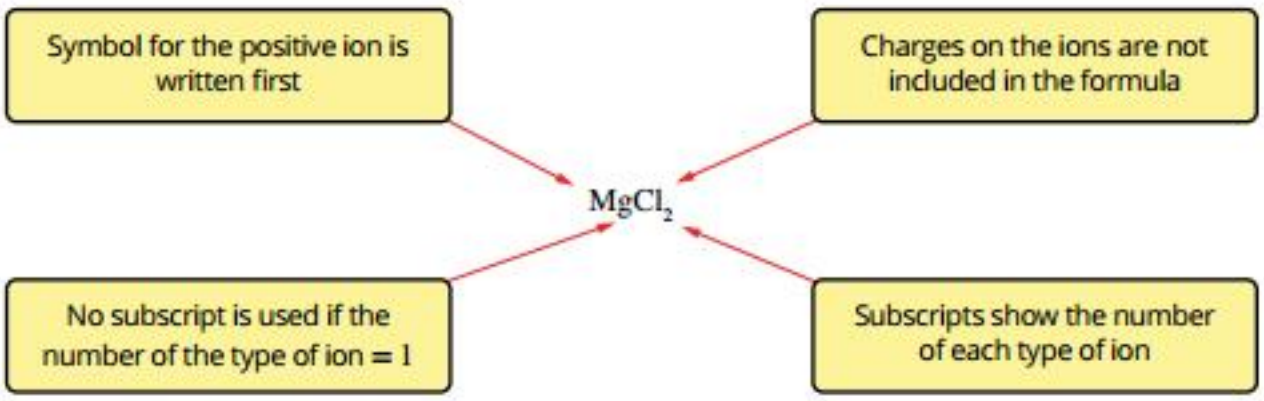

Symbol for the positive ion is written first
Charges on the ions are not included in the formula
$MgCl_2$
No subscript is used if the number of the type of ion = 1
Subscripts show the number of each type of ion

FIGURE 7.3.2 Summary of the information provided by a chemical formula

Worked example 7.3.1

STEPS IN WRITING A CHEMICAL FORMULA

Determine the chemical formula of the ionic compound formed between zinc and nitride ions. You may need to refer to Tables 7.3.1 and 7.3.2 on page 138.	
Thinking	**Working**
Write the symbol and charge of the two ions forming the ionic compound.	Zn^{2+} and N^{3-}
Calculate the lowest common multiple of the two numbers in the charges of the ions.	$2 \times 3 = 6$
Calculate how many positive ions are needed to equal the lowest common multiple.	three Zn^{2+} ions
Calculate how many negative ions are needed to equal the lowest common multiple.	two N^{3-} ions
Use the answers from the previous two steps to write the formula for the ionic compound using subscripts to show the number of ions. Write the symbol of the positive ion first.	Zn_3N_2

➤ Try yourself 7.3.1

STEPS IN WRITING A CHEMICAL FORMULA

Determine the chemical formula of the ionic compound formed between barium and fluoride ions. You may need to refer to Tables 7.3.1 and 7.3.2 on page 138.

NAMING SIMPLE IONIC COMPOUNDS

There are some conventions that are followed when naming ionic compounds.

- The first part of the name is the name of a positively charged metal ion (cation). This is the same as the name of the metal. For example, the cation of a sodium atom is called a sodium ion; the cation of an aluminium atom is called an aluminium ion.
- For simple **monatomic** anions that are formed from only one atom, the second part of the name is the non-metal ion (anion). The name of this ion is similar to that of the atom, but ends in '-ide'. For example, the anion of a chlorine atom is chloride; the anion of an oxygen atom is called oxide. (Some names for more complex ions are derived differently and are described at the end of this module.)

Worked example 7.3.2

STEPS IN WRITING THE NAME OF AN IONIC COMPOUND

Determine the name of Zn_3N_2 (without using Tables 7.3.1 and 7.3.2).	
Thinking	**Working**
Write the name of the cation (the first element in the formula) with a Roman numeral if required.	zinc
Write the name of the second element (non-metal) in the formula.	nitrogen
Change the ending of the non-metal element to 'ide'.	nitride
Write the two names together (with a space between each word).	zinc nitride

➤ Try yourself 7.3.2

STEPS IN WRITING THE NAME OF AN IONIC COMPOUND

Determine the name of $CuBr_2$ (without using Tables 7.3.1 and 7.3.2).

FORMULAS CONTAINING POLYATOMIC IONS

Simple monatomic ions contain only one atom. However, other ions contain atoms of two or more elements. These ions are called **polyatomic ions**.

In polyatomic ions:

- different atoms are present, combined in a fixed ratio
- the group of atoms behaves as a single unit with a specific charge
- subscripts are used to indicate the number of each kind of atom in the ion.

For example, a carbonate ion (CO_3^{2-}) contains one carbon atom and three oxygen atoms covalently bonded to form an ion. The carbonate ion has a charge of 2–. Other common polyatomic ions are nitrate (NO_3^-), hydroxide (OH^-) and phosphate (PO_4^{3-}). The formulas of common polyatomic ions can be seen in Table 7.3.3.

TABLE 7.3.3 Common polyatomic cations and anions

Charge			
1+	1–	2–	3–
ammonium, NH_4^+ hydronium, H_3O^+	cyanide, CN^- dihydrogen phosphate, $H_2PO_4^-$ ethanoate, CH_3COO^- hydrogen carbonate, HCO_3^- hydrogen sulfide, HS^- hydrogen sulfite, HSO_3^- hydrogen sulfate, HSO_4^- hydroxide, OH^- nitrite, NO_2^- nitrate, NO_3^- permanganate, MnO_4^-	carbonate, CO_3^{2-} chromate, CrO_4^{2-} dichromate, $Cr_2O_7^{2-}$ hydrogen phosphate, HPO_4^{2-} oxalate, $C_2O_4^{2-}$ sulfite, SO_3^{2-} sulfate, SO_4^{2-}	phosphate, PO_4^{3-}

If more than one polyatomic ion is required in a formula to balance the charge, then it is placed in brackets with the required number written as a subscript after the brackets. Some examples are:

- magnesium nitrate, $Mg(NO_3)_2$. The brackets and subscript show that for every Mg^{2+} ion, there are two nitrate (NO_3^-) ions present in the lattice.

- iron(III) sulfate, $Fe_2(SO_4)_3$. The (III) in the formula means the cation has a 3+ charge. The brackets and subscripts show that for every three sulfate ions (SO_4^{2-}), there are two iron(III) ions present in the lattice.

The diagrams in Figure 7.3.3 show the formation of these two compounds containing polyatomic ions.

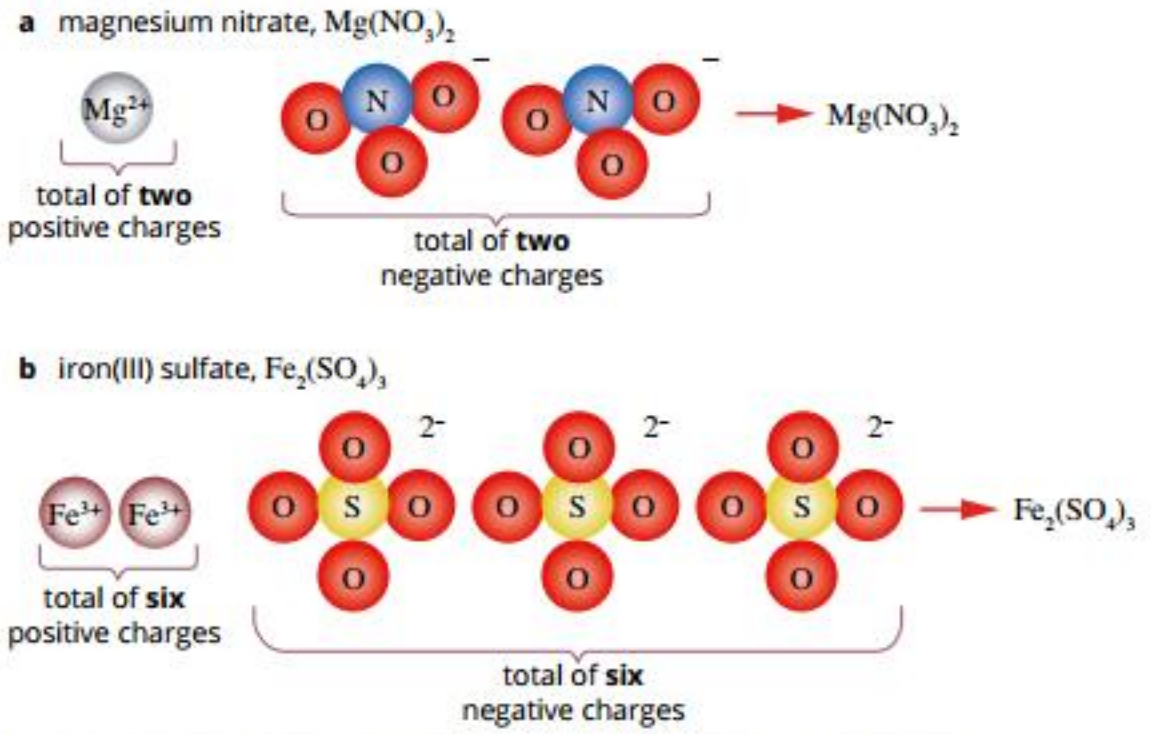


FIGURE 7.3.3 The chemical formulas of ionic compounds containing polyatomic ions

Note that brackets are not required for the formula of sodium nitrate, $NaNO_3$, where there is only one NO_3^- ion present for each sodium ion.

> Polyatomic ions are made up of two or more different atoms that have an overall charge. They need to be written within brackets if there is more than one present in the chemical formula. Subscripts are used to indicate the ratio of ions in the crystal lattice.

Worked example 7.3.3

STEPS IN WRITING A CHEMICAL FORMULA INCLUDING POLYATOMIC IONS

Determine the chemical formula of the ionic compound formed between magnesium and nitrate ions. You may need to refer to Table 7.3.3 on page 140.	
Thinking	**Working**
Write the symbol and charge of the two ions forming the ionic compound.	Mg^{2+} and NO_3^-
Calculate the lowest common multiple of the two numbers in the charges of the ions.	$2 \times 1 = 2$
Calculate how many positive ions are needed to equal the lowest common multiple.	one Mg^{2+} ion
Calculate how many negative ions are needed to equal the lowest common multiple.	two NO_3^- ions
Use the answers from the previous two steps to write the formula for the ionic compound using subscripts to show the number of ions. Write the symbol of the positive ion first. Use brackets around a polyatomic ion when adding a subscript. (Note that 1 is not written as a subscript.)	$Mg(NO_3)_2$

➤ Try yourself 7.3.3

STEPS IN WRITING A CHEMICAL FORMULA INCLUDING POLYATOMIC IONS

Determine the chemical formula of the ionic compound formed between zinc and hydroxide ions. You may need to refer to Table 7.3.3 on page 140.

Naming ionic compounds containing polyatomic ions

When naming ionic compounds containing polyatomic ions, we follow the same approach as above: name the cation first, followed by the anion. However, Table 7.3.3 on page 140 shows that the names of polyatomic anions usually do not end in 'ide'. Polyatomic anions containing oxygen will end in '-ite' or '-ate'. The name of the ion with the smaller number of oxygen atoms usually ends in '-ite' and the one with the larger number of oxygen atoms usually ends in '-ate'. For example, the NO_2^- ion is called a nitrite ion and the NO_3^- ion is called a nitrate ion.

There are two polyatomic cations in Table 7.3.3 on page 140 —the ammonium ion, NH_4^+, and the hydronium ion, H_3O^+. These ions are formed during acid–base reactions. An ammonium ion is formed when an ammonia molecule, NH_3, bonds to a hydrogen ion, H^+, and a hydronium ion is formed when a water molecule, H_2O, bonds to a hydrogen ion, H^+.

Some ions that are widely used have a common name. The common name for the ethanoate ion is acetate, and the common name for the hydrogen carbonate ion is bicarbonate.

7.3 Review

SUMMARY

- When determining the formula of an ionic compound, the total number of positive charges on the metal ion(s) must equal the total number of negative charges on the non-metal ion(s).
- Ions that contain two or more atoms of different elements are called polyatomic ions.
- When writing formulas of ionic compounds:
  - the symbol for the positively charged ion is written first
  - subscripts are used to indicate the number of each ion in the formula
  - the charges on the ions are not included in the balanced formula
  - if a chemical formula contains more than one polyatomic ion, the formula of the ion is placed in brackets, with the number of ions written as a subscript after the brackets.
- When naming ionic compounds, the name of the cation is written first, followed by the name of the anion.
- The name of a polyatomic anion containing oxygen will usually end in '-ite' or '-ate'.

KEY QUESTIONS

Describe

1 Use the information provided in Tables 7.3.1 and 7.3.2 on page 138 to name the ionic compounds with the following formulas.

a LiCl
b CaO
c MgS
d K_2O
e NaF
f AgI
g Ca_3N_2
h CuF
i $PbCl_4$

2 Use the information in Tables 7.3.1 and 7.3.2 on page 138 to write formulas for the following ionic compounds.

a sodium iodide
b potassium bromide
c zinc chloride
d potassium oxide
e barium bromide
f chromium(III) iodide
g silver bromide
h copper(I) oxide
i calcium oxide
j aluminium sulfide

Apply

3 Listed below are pairs of metal and non-metal ions. Determine the ratio of the metal ion to the non-metal ion when they combine to form ionic compounds.

a K^+ and S^{2-}
b Al^{3+} and F^-
c Ca^{2+} and N^{3-}
d Al^{3+} and P^{3-}
e Mg^{2+} and Cl^-

4 Explain why the formula $CuOH_2$ is not the correct formula for copper(II) hydroxide. In your answer, you should include the correct formula for the compound.

5 Use the information provided in Table 7.3.1 on page 138 and Table 7.3.3 on page 140 to name the following ionic compounds.

a $Mg(OH)_2$
b Na_2CO_3
c $FePO_4$
d $CuSO_4$
e $Ba(NO_3)_2$
f $CuHCO_3$
g $Fe(CH_3COO)_2$
h NH_4NO_3
i Na_2HPO_4

6 Use the information provided in Tables 7.3.1 and 7.3.2 on page 138 and Table 7.3.3 on page 140 to determine the chemical formulas for the following ionic compounds.

a sodium carbonate
b calcium hydrogensulfate
c copper(II) nitrate
d calcium hydroxide
e aluminium hydrogencarbonate
f potassium phosphate
g ammonium sulfate
h zinc cyanide

7 In Question **6**, there were four compounds in which there were twice as many anions as cations in the formula unit of the compound. Write the formulas of these four compounds.

Analyse

8 Using the periodic table on page 132 and without referring to Tables 7.3.1 and 7.3.2, determine the formulas for the ionic compounds made from the following metals and non-metals.

a potassium and chlorine
b calcium and iodine
c bromine and aluminium
d oxygen and magnesium
e rubidium and phosphorus
f nitrogen and lithium

9 Consider the formulas for ammonium hydrogen phosphate and aluminium carbonate. Summarise in the tables below the number of atoms of each element found in the formula unit of each of the compounds. The first one has been started for you.

Compound: ammonium hydrogen phosphate	
Formula:	
Element	**Number of atoms in formula unit**
N	2
H	
P	1
O	

Compound: aluminium carbonate	
Formula:	
Element	**Number of atoms in formula unit**

10 Using the periodic table on page 132 and without referring to Tables 7.3.1, 7.3.2 or 7.3.3, consider each of the following ionic compounds. The formulas that have been written for them are incorrect.

i Explain why each formula is incorrect.
ii Write the correct formula for each ionic compound.

a ammonium sulfide, $(NH_4)_2SO_4$
b copper(II) nitrate, $CuNO_3$
c zinc phosphate, Zn_2PO_4

11 A_2B is an ionic compound. Both of the ions in A_2B have the same electron configuration as an argon atom. Determine the identity of A_2B. Explain your answer.

Chapter review

07

KEY TERMS

anion
aqueous
boiling point
brittle
cation
ceramic
ceramic insulator
charge imbalance
chemical formula
conductivity
crystal lattice
current
dissolve
electrode
electrolyte
electron transfer diagram
electronegativity
electrostatic attraction
element
empirical formula
formula unit
insoluble
ion
ionic bond
ionic compound
melting
melting point
metal ion
molecular formula
monatomic
non-metal ion
octet rule
polyatomic ion
soluble
three-dimensional lattice
transition metal
valence shell

KEY QUESTIONS

Describe

1 Describe what the subscripts in the formula of an ionic compound tell you about the cations and anions in the compound.

2 Use Table 7.3.3 on page 140 to identify:
- **a** the anion containing the most atoms
- **b** the anion with the greatest charge.

3 Complete this summary table of properties of ionic compounds and the information this provides about their structure.

Property	What this tells us about structure
	The forces of attraction between the particles are strong.
hard, brittle crystals	
does not conduct electricity in the solid state	No free-moving charged particles are present in the solid.
conducts electricity in the molten state or in an aqueous solution	
	The strength of the interaction of ions with water particles varies, as does the strength of the bonds within the lattice.

4 Use the ionic bonding model to explain the following properties of ionic compounds.
- **a** They generally have high melting points.
- **b** They are hard and brittle.
- **c** They do not conduct electricity in the solid state, but will conduct when molten or dissolved in water.

5 Identify which of the following are likely to be ionic substances. More than one answer may be correct.
- **A** sodium bromide
- **B** magnesium chloride
- **C** silicon dioxide
- **D** phosphorus trichloride

6 Which one of the following compounds contains an anion that has a 2– charge?
- **A** $CaCl_2$
- **B** $AlBr_3$
- **C** Na_2O
- **D** $Pb(OH)_2$

Apply

7 Determine which of the following is *not* a property of solid ionic compounds.
- **A** poor conductor of electricity
- **B** high melting point
- **C** soluble in water
- **D** ductile

8 Which of the following explains the change in electrical conductivity between solid ionic compounds and molten ionic compounds?
- **A** the effect of heat in removing electrons from ions
- **B** water molecules carrying charge
- **C** ions becoming free to move (carrying charge)
- **D** electrons passing through the lattice structure

9 Which of the following options correctly identifies the charge on M in MCl_2?
- **A** 2+
- **B** 1+
- **C** 1–
- **D** 2–

10 Determine whether the following properties relate to metallic lattices only, ionic lattices only, or both metallic and ionic lattices.

- **a** They contain both positively and negatively charged particles.
- **b** The lattice is held together by forces of attraction between positively and negatively charged particles.
- **c** They are hard.
- **d** They are brittle.
- **e** They conduct electricity in the molten state.

11 Name the ionic compounds with the following chemical formulas.

- **a** $(NH_4)_2CO_3$
- **b** $Cu(NO_3)_2$
- **c** $CrBr_3$

12 Which of the following correctly describes what happens to the structure of solid sodium chloride when it melts?

- **A** The cations and anions lose their charge and become atoms.
- **B** The cations and anions separate and the lattice structure is destroyed.
- **C** Molecules of sodium chloride separate from the ionic lattice.
- **D** The ions move rapidly and spread throughout the container, filling the entire three-dimensional space.

13 Use the electron configurations and a balanced chemical equation to show the electron transfer that occurs when:

- **a** lithium reacts with chlorine
- **b** magnesium reacts with fluorine
- **c** potassium reacts with sulfur
- **d** magnesium reacts with nitrogen.

14 Explain why elements in group 17 of the periodic table are likely to forms ions with a 1– charge.

15 Write the chemical formula for the ionic compound formed in each of the following reactions.

- **a** potassium and bromine
- **b** magnesium and iodine
- **c** calcium and oxygen
- **d** aluminium and fluorine
- **e** calcium and nitrogen

16 Write the chemical formula that represents each of the following ionic compounds. You may need to refer to Tables 7.3.1 and 7.3.2 on page 138.

- **a** copper(I) chloride
- **b** silver oxide
- **c** lithium nitride
- **d** potassium iodide

17 Complete the table below by writing the chemical formulas for four ionic compounds formed using combinations of cations and anions as shown.

	K^+	Ca^{2+}
F^-		
N^{3-}		

18 Refer to the diagrams shown in Figure 7.3.3 on page 141 and draw a diagram that shows the formation of magnesium sulfate.

19 Draw a concept map to show the connection between the following terms: metal, non-metal, atom, valence electron, anion, cation, electrostatic attraction, ionic compound.

Analyse

20 An ionic compound is formed between an unknown metal ion, M^{x+}, and the sulfate ion. The formula of the compound is $M_2(SO_4)_3$. Which of the following ions could be the metal ion, M^{x+}?

- **A** Mg^{2+}
- **B** Na^+
- **C** Al^{3+}
- **D** Ca^{2+}

21 Describe the properties of ionic compounds that can be explained by the regular arrangement of ions in the lattice.

22 A student has described the formation of an ionic compound in the following two sentences.

The metal atom loses its valence electrons to form a positive ion and the non-metal atom gains those electrons to form a negative ion. The metal ion and the non-metal ion then pair up to form a molecule.

This description contains several misunderstandings about the formation of ions and the structure of ionic compounds. Analyse the student's description and explain their misunderstandings.

23 Apply the concept of a formula unit to explain why the chemical formula of an ionic compound is not just the actual number of atoms in the compound.

24 The electron configurations of some metallic and non-metallic elements are given below. (The symbols shown for the elements are not their real ones.) Write formulas for the compounds they are most likely to form if they react together. The first example has been done for you.

- **a** A: $[He]2s^1$ B: $[He]2s^22p^4$ A_2B
- **b** C: $[Ne]3s^23p^1$ D: $[He]2s^22p^5$
- **c** E: $[Ne]3s^23p^4$ F: $[Ar]4s^2$
- **d** G: $[He]2s^22p^3$ H: $[Ar]4s^1$
- **e** K: $[Ne]2s^2$ L: $[He]2s^22p^4$

25 Represent the transfer of electrons between the following metal and non-metal atoms using an equation and write a second equation showing the formation of the ionic compound.
- **a** magnesium and chlorine atoms
- **b** aluminium and oxygen atoms

26 Use the information provided in Tables 7.3.1 and 7.3.2 on page 138 and Table 7.3.3 on page 140 to write formulas for the following ionic compounds.
- **a** iron(III) oxide
- **b** copper(II) sulfide
- **c** chromium(III) sulfate
- **d** iron(II) carbonate
- **e** lead(II) nitrate
- **f** lead(IV) dichromate
- **g** tin(II) ethanoate

27 A student researched the properties of three different ionic compounds: calcium bromide ($CaBr_2$), calcium chloride ($CaCl_2$) and magnesium oxide (MgO).
The student found that the melting points of the compounds are as shown in the table below.
If the three compounds were all heated to 800°C, complete the table to indicate whether each compound would conduct electricity.

Compound	Melting point (°C)	Electrical conductivity (yes/no)
calcium bromide	730	
calcium chloride	772	
magnesium oxide	2852	

28 The elements X, Y and Z form ionic compounds when they react with other elements. The following compounds are formed: Ca_3X_2, Y_2CO_3 and Al_2Z_3.
- **a** Determine the charge on the ion formed by:
  - **i** element X
  - **ii** element Y
  - **iii** element Z
- **b** Use these charges on the ions to deduce correct chemical formulas for the:
  - **i** sulfate salt of Y
  - **ii** potassium salt of Z
  - **iii** ionic compound formed between X and Y
  - **iv** ionic compound formed between Y and Z

Interpret

29 The melting point of sodium chloride is 801°C, whereas the melting point of magnesium oxide is 2800°C.
- **a** Identify the particles present in the two solids.
- **b** Which solid has the stronger forces between its particles?
- **c** By considering the charge on each ion, suggest a reason for the difference in the melting points of sodium chloride and magnesium oxide.

30 The formula of sodium perchlorate is $NaClO_4$ and that of silver arsenate is Ag_3AsO_4. Using this information, propose the formula for the following.
- **a** calcium perchlorate
- **b** aluminium arsenate
- **c** iron(III) perchlorate
- **d** copper(II) arsenate

31 Propose an experiment you could carry out to demonstrate each of the following properties of the compounds given. In each case:
  - **i** sketch the equipment you would use
  - **ii** describe what you would expect to observe.
- **a** Solid magnesium chloride does not conduct electricity.
- **b** Dissolved sodium chloride does conduct electricity.
- **c** Solid sodium chloride is hard and brittle.

32 A student analyses the structure and bonding in a metal and an ionic compound. From this analysis, the student makes the statements below.
- **a** Metals and ionic compounds both contain positive ions in a regular arrangement.
- **b** In metals and ionic compounds, there is attraction between one particle and all the neighbouring particles of opposite charge.
- **c** In metals and ionic compounds, there will be forces of repulsion between particles with like charges.
- **d** A metal will conduct electricity, whereas a solid ionic compound will not, because electrons are much smaller than negative ions.

Judge whether you agree or disagree with each statement. Provide reasons for your decisions.

CHAPTER

08 Covalent compounds

Although there are fewer non-metals than metals in the periodic table, the atoms of non-metals form a much larger number of compounds than metals. Water, carbon dioxide, caffeine, sugar and cooking oil are just a few examples of common compounds formed from non-metals.

At the end of this chapter, you will understand that covalent bonding exists in compounds and elements formed from two or more non-metallic atoms. When non-metals bond, their atoms share electrons to gain stable valence electron shells. Most substances formed from non-metallic elements have relatively low melting and boiling points and are composed of small molecules.

Other substances, such as carbon, form giant covalent networks of atoms, which result in quite different chemical and physical properties.

Syllabus subject matter

Topic 1 • Properties and structure of atoms

■ INTRODUCTION TO BONDING

- Determine Lewis (electron dot) structure of molecules and ions showing all valence electrons for up to four electron pairs for each atom. **8.2**
- Identify the numbers of bonding and lone pairs of electrons around each atom in a molecule. **8.2**
- Determine the formula and IUPAC name of ionic and molecular compounds. **8.3**

Topic 2 • Properties and structure of materials

■ BONDING AND PROPERTIES

- Describe the properties of ionic, covalent and metallic compounds, e.g. melting and boiling point, thermal and electrical conductivity, strength and hardness.* **8.1**
- Explain that the type of bonding within ionic, metallic and covalent substances determines their physical properties.* **8.1**
- Explain the properties of covalent compounds by modelling covalent bonding as the sharing of an electron pair in the region between two nuclei with a strong electrostatic force of attraction between both nuclei. **8.2**
- Discriminate between covalent molecules, giant covalent networks and allotropes of carbon. **8.4**
- Explain that hydrocarbons, including alkanes (saturated), alkenes (unsaturated) and benzene, have different chemical properties that are determined by the nature of the bonding within the molecules. **8.2**
- Analyse data to determine the properties, structure and bonding of ionic, covalent and metallic compounds.* **8.2**

*The greyed-out section of this dot point is addressed explicitly in another chapter.

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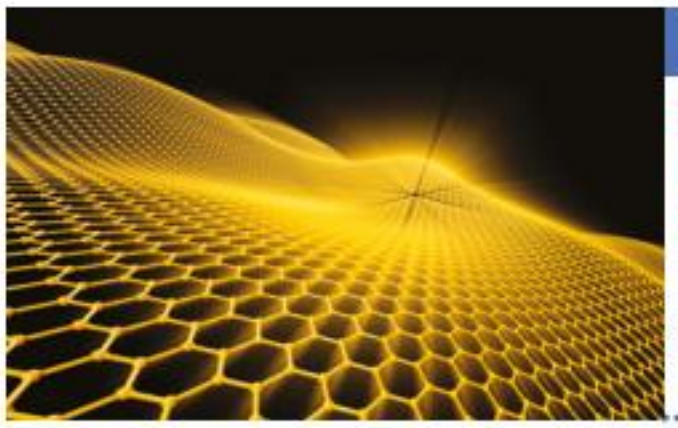
8.1 Properties of covalent substances



BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe some of the properties common to covalent substances
- define what a molecule is
- recognise the differences between intramolecular bonds and intermolecular forces
- explain that intramolecular bonds and intermolecular forces in covalent substances determine their physical properties.

In Chapter 6, you saw that the bonding between atoms in metallic elements is called metallic bonding. In Chapter 7, you saw that when metal atoms combine with atoms of non-metallic elements, the compounds contain another form of bonding, ionic bonding. In this chapter, you will look at the chemical bonding that occurs when atoms of non-metals combine.

PROPERTIES OF COVALENT SUBSTANCES

Compounds formed by non-metallic elements tend to be molecular compounds; that is, they form molecules, like water. They are also called **covalent compounds**. The properties of covalent compounds can tell you a lot about their chemical structures. Table 8.1.1 lists some of the properties of a range of common substances. The substances chosen include metallic elements, non-metallic elements, ionic compounds and molecular compounds. The information in Table 8.1.1 is useful because it allows you to:

- identify the characteristic properties of each category of substances. For example, metals conduct electricity as solids and liquids.
- deduce information about the chemical structures of these substances. If a substance has a high melting point, the bonding between particles must be strong. If a substance conducts electricity, it must contain charged particles that are free to move.

TABLE 8.1.1 Properties of some common metals, ionic compounds and covalent substances

Substance	Formula	Melting point (°C)	Boiling point (°C)	Conducts electricity as a solid?	Conducts electricity as a liquid?
ammonia	NH_3	−77	−33	no	no
copper	Cu	1084	2562	yes	yes
chlorine	Cl_2	−102	−34	no	no
copper(II) chloride	$CuCl_2$	498	993	no	yes
nitrous oxide	N_2O	−90	−88	no	no
sodium chloride	NaCl	801	1413	no	yes
oxygen	O_2	−219	−183	no	no
water	H_2O	0	100	no	no

Table 8.1.1 shows some of the properties of common substances.

- Metals such as copper have high melting points and conduct electricity as solids and as liquids. As you saw in Chapter 6, this indicates that strong bonds exist in metals and that they contain charged particles (delocalised electrons) that are free to move in the metal.
- The ionic compounds copper(II) chloride and sodium chloride have high melting points and conduct electricity as liquids, but not as solids. In Chapter 7, you learnt that ionic solids have strong bonds and that they contain charged particles (ions) that are free to move in a liquid form, but not in a solid form.
- The non-metallic elements chlorine and oxygen form molecules. They have low melting points and do not conduct electricity. The same is true for the molecular compounds ammonia, nitrous oxide and water. Two conclusions about bonding in covalent substances that can be drawn from these properties are shown in Figure 8.1.1.

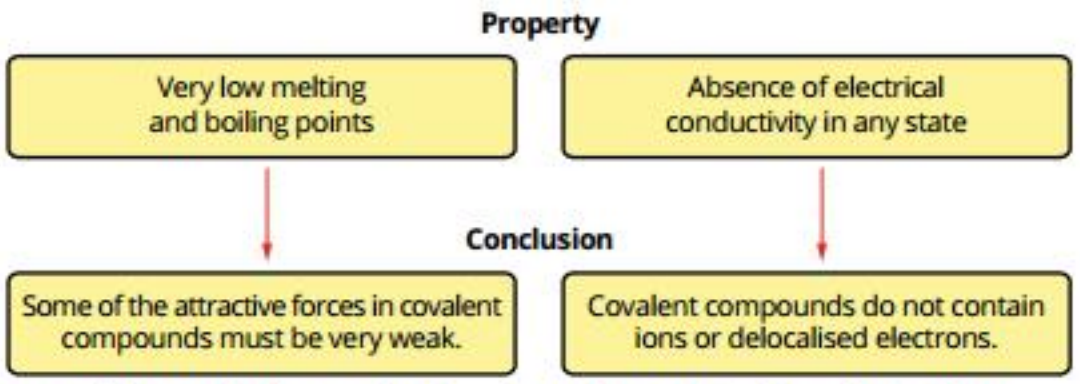
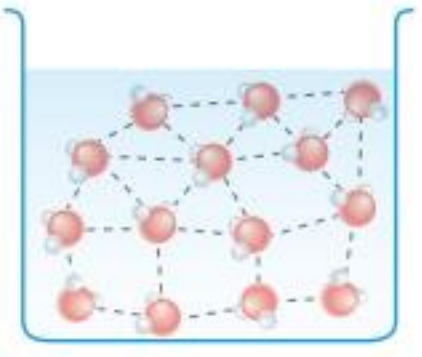

Property
Very low melting and boiling points
Absence of electrical conductivity in any state
Conclusion
Some of the attractive forces in covalent compounds must be very weak.
Covalent compounds do not contain ions or delocalised electrons.

FIGURE 8.1.1 These conclusions can be drawn from the properties of covalent substances.

Molecules

You gain further insight into the chemical structure of covalent substances by considering what happens when you boil water in a beaker. For example, a representation of liquid water is provided in Figure 8.1.2, showing that each water **molecule** contains two hydrogen atoms bonded to one oxygen atom. In between the molecules are weak attractive forces that are responsible for keeping all the molecules together.



Water in a beaker contains two types of bonds:
1. the bonds between hydrogen and oxygen atoms within each water molecule
2. the bonds holding one molecule of water to another.

FIGURE 8.1.2 This representation shows the attractive forces between water molecules in a beaker.

The particles of water are **molecules** because they are definite and discrete groups of atoms chemically bonded together. The atoms in molecules are typically non-metallic atoms bonded to other non-metallic atoms. Molecules can be found in elements as well as compounds. The element oxygen, for example, forms O_2 molecules—two non-metallic oxygen atoms bonded together. O_2 is referred to as a **molecular element** as it contains only one type of atom. Water, on the other hand, is referred to as a **molecular compound** (containing more than one element) with a **molecular formula** of H_2O.

When liquid water boils (Figure 8.1.3), some water molecules gain enough energy to break free from the others and escape from the surface of the liquid as water vapour. The water vapour is still molecules of water, so the bonds between atoms within each molecule of water (the **intramolecular bonds**) have not been broken. Instead, it is the **intermolecular forces** between the water molecules that have been disrupted. This indicates that the intramolecular bonds within molecules are much stronger than the intermolecular forces between molecules. The types of intermolecular forces that exist and the factors that determine their strength will be covered in more detail in Chapter 11.

i Heating a covalent molecular substance to its melting or boiling point disrupts its intermolecular forces, allowing it to change state from solid to liquid or from liquid to gas, respectively.

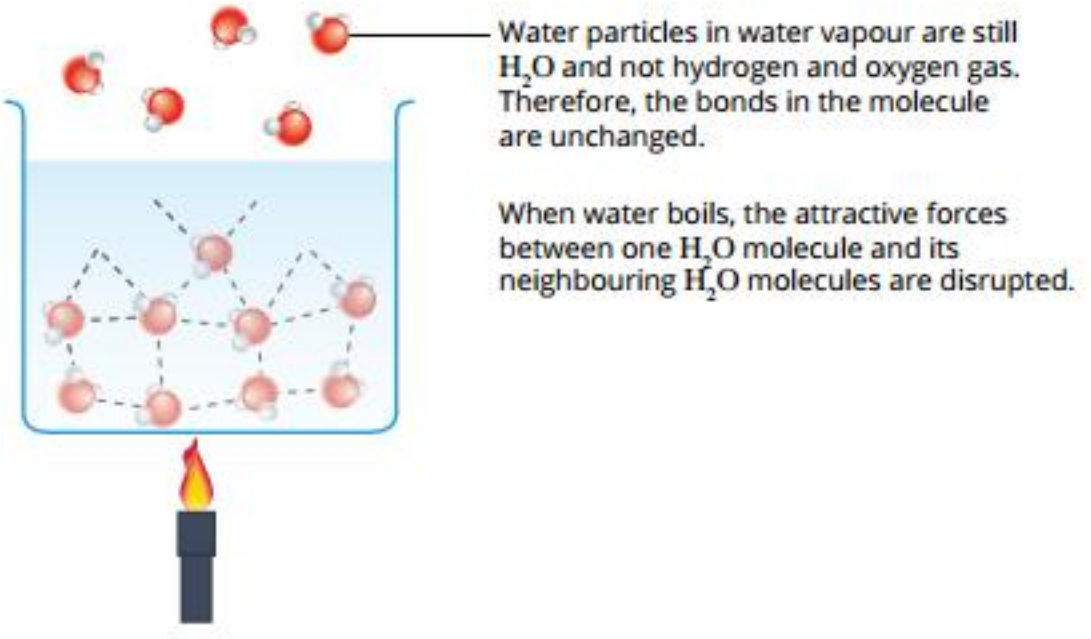

Water particles in water vapour are still H_2O and not hydrogen and oxygen gas. Therefore, the bonds in the molecule are unchanged.
When water boils, the attractive forces between one H_2O molecule and its neighbouring H_2O molecules are disrupted.

FIGURE 8.1.3 Changes in the bonding of water occur when it starts to boil.

8.1 Review

SUMMARY

- Many substances contain only non-metal atoms. Some of these substances are elements, while others are compounds. These substances are known as covalent substances.
- Covalent substances usually have low boiling points and do not conduct electricity.
- Many covalent substances are composed of molecules. A molecule is a definite and discrete group of atoms chemically bonded together. The atoms in molecules are non-metallic atoms bonded to other non-metallic atoms.
- In molecular compounds, the bonds within the molecules holding the atoms together are called intramolecular bonds and the attractive forces between molecules are called intermolecular forces.
- The melting and boiling points of covalent substances depend on the attractive forces between molecules. Generally, molecular substances have low melting and boiling points. This indicates that they have weak attractive forces between molecules.
- In general, covalent substances do not conduct electricity because they do not contain free-moving charged particles (neither delocalised electrons nor ions).

KEY QUESTIONS

Describe

1 Identify each of the following as a covalent compound, ionic compound, element, or covalent molecular element.

a $CaSO_4$
b N_2O_5
c H_2
d Cu
e $FeCl_2$
f I_2

2 Define the term 'molecule'.

3 Referring to Table 8.1.1 on page 148, identify the physical properties that are linked to the strength of the bonding or attractive forces between particles.

4 Identify whether intramolecular bonds or intermolecular forces are disrupted when a covalent molecular substance is boiling.

Apply

5 Explain why the compound aluminium oxide, Al_2O_3, is not considered a covalent molecular compound.

6 Refer to Table 8.1.1 on page 148 to answer the following questions.

a Identify all the covalent molecular substances.
b Identify the physical property that distinguishes a covalent molecular compound from a metal or an ionic compound.

Analyse

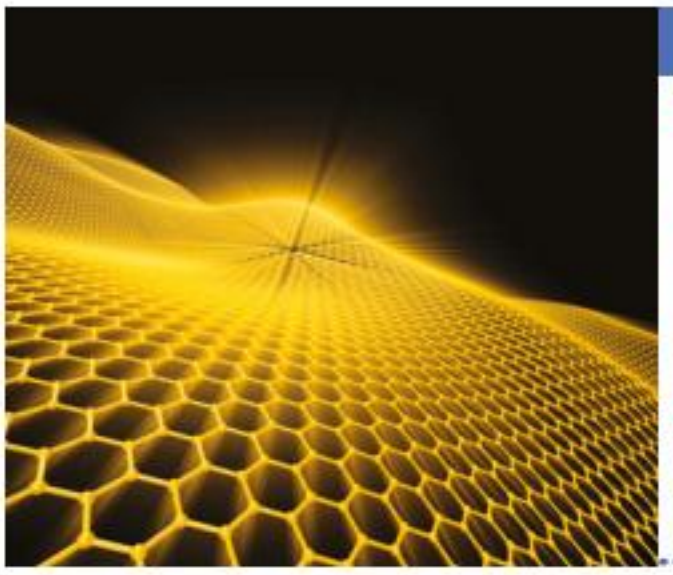
7 Sodium chloride (NaCl) has a boiling point of 801°C and ammonia (NH_3) has a boiling point of –77°C.

a Identify the particles found in each substance.
b Explain the differences between the boiling points of sodium chloride and ammonia.

8 Assess the relative strengths of the intermolecular forces in the covalent molecular compounds methane, CH_4 (b.p. –161°C), and water, H_2O (b.p. 100°C), given the differences in their boiling points.

9 When sugar (sucrose, $C_{12}H_{22}O_{12}$) is heated gently, it turns into a clear liquid. If the liquid is heated strongly, it turns black and a gas is produced. Describe what is happening to the bonds in sugar when it is heated gently, and when it is heated strongly. Use the terms 'intramolecular bonds' and 'intermolecular forces' in your answer.

8.2 Covalent bonding



BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that covalent bonds involve sharing of valence electrons between atoms
- recall that non-metallic atoms can bond with other non-metallic atoms via single, double or triple bonds
- identify trends in bond lengths and bond strengths depending on whether covalent bonds between atoms are single, double or triple
- determine the Lewis structure of polyatomic molecules and ions
- identify the number of bonding pairs and lone pairs (non-bonding pairs) of electrons in a molecule or ion.

This module examines several simple molecules to help you to understand the concept of a **covalent bond**, which is formed when non-metallic atoms share electrons. Using your knowledge of the valence shell electron arrangements of non-metallic atoms, you will be able to predict the molecules that can be formed from non-metallic elements.

COVALENT BONDS

In Chapter 3, you saw that atoms of main group elements become more stable if they obtain a valence shell of eight electrons by combining with other atoms (the **octet rule**).

Commonly, when atoms of non-metals combine, electrons are shared, so that each atom has eight electrons in its valence shell. Molecules formed in this way are more stable than the separate atoms. The major exception to the octet rule is hydrogen, which can only accommodate a maximum of two electrons in its valence shell.

Non-metallic atoms have a relatively high number of electrons in their valence shells and they tend to share rather than to transfer electrons. A covalent bond is a strong electrostatic attraction between two atoms that occurs when one or more pairs of electrons are shared between two nuclei. As discussed in the previous module, covalent bonds are the intramolecular bonds found within molecules.

Single covalent bonds

When atoms share two electrons, one from each atom, the covalent bond formed is called a **single covalent bond**. Two examples of substances that contain single bonds are hydrogen and chlorine.

Hydrogen

Hydrogen atoms have one electron. The valence shell of a hydrogen atom can hold a maximum of two electrons. A hydrogen atom can bond to another hydrogen atom by sharing their individual electrons to form a molecule of H_2, as shown in Figure 8.2.1.

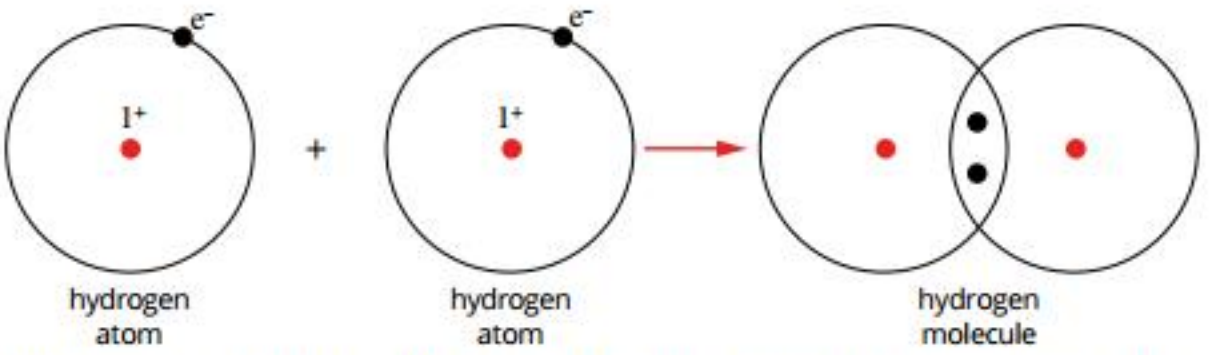


FIGURE 8.2.1 A covalent bond is formed when two hydrogen atoms share two electrons, one from each atom.

In the molecule that is formed:

- two hydrogen atoms share one electron each to form a single covalent bond
- the atoms of hydrogen are now strongly bonded together by two electrons (an electron pair) in their valence shells.

The hydrogen molecule can be represented by the molecular formula, H_2. Molecules that contain two atoms are called **diatomic molecules**.

Two alternative ways of representing a hydrogen molecule are shown in Figure 8.2.2.

In a hydrogen molecule, the two electrons are attracted to both nuclei (protons) of the H_2 structure. This means the two electrons will spend most of their time between the two nuclei instead of orbiting their original nuclei. Even though the protons in the two nuclei still repel each other (remember, like charges repel), their electrostatic attraction to the electrons (which are closer) keeps the molecule held together.

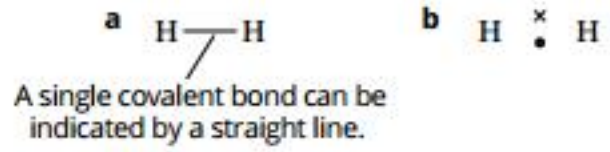


FIGURE 8.2.2 Two representations of a hydrogen molecule: (a) the single covalent bond is shown as a single straight line or (b) the electrons in the covalent bond are represented using a dot and a cross. In this case, the dot and cross represent electrons that originated from two different hydrogen atoms.

This model of a hydrogen molecule is consistent with the observed properties of hydrogen gas. The covalent bonds within the molecules are strong, but the intermolecular forces between hydrogen molecules are weak. This explains the low melting point of –259°C for hydrogen. Hydrogen does not conduct electricity as it does not contain ions or delocalised electrons.

Hydrogen is an example of a covalent molecular substance.

Chlorine

A chlorine atom has a condensed electron configuration of [Ne]$3s^2 3p^5$, which means that it has seven electrons in its valence shell. It requires one more electron to achieve a stable octet of electrons in its valence shell. Two chlorine atoms can share one electron each to form a molecule of chlorine with a single covalent bond. As a result, both atoms gain valence shells of eight electrons, as shown in Figure 8.2.3. This is an example of the application of the octet rule.

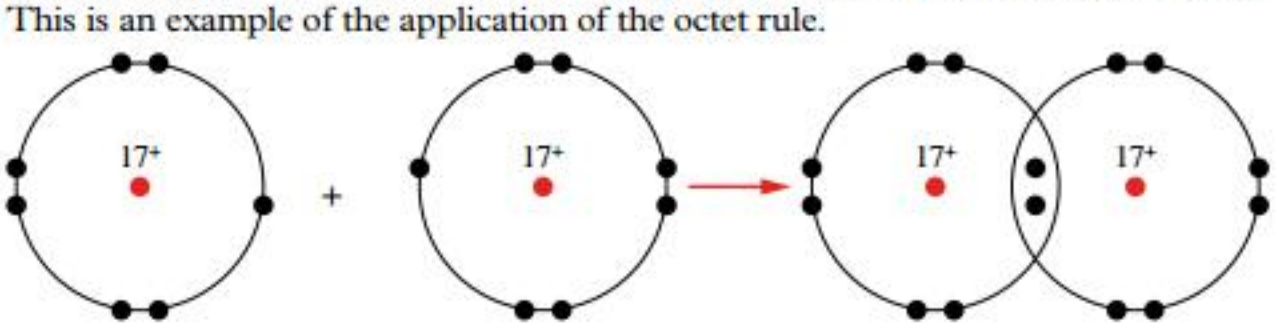


FIGURE 8.2.3 Two chlorine atoms share one electron each to form a chlorine molecule. Note that only valence shell electrons are shown in these diagrams.

Lewis structures

Chemists often use **Lewis structures** (also known as **electron dot diagrams**) to represent molecules. Lewis structures show just the valence shell electrons of atoms, as only these electrons are involved in bonding.

Figure 8.2.4 shows examples of the Lewis structure for a molecule of chlorine. In a Lewis structure, a pair of electrons can be represented by dots, crosses or a line. Lewis structures can even be drawn using combinations of all three ways of representing electron pairs. However, the preferred Lewis structure uses a straight line to represent a bonding pair of electrons.

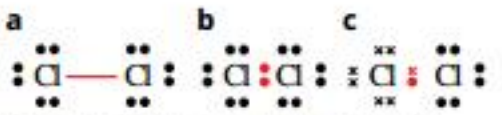


FIGURE 8.2.4 Three examples of Lewis structures for a chlorine molecule showing the bonding pair and lone pairs (non-bonding pairs) of electrons. The bonding pair is shown in red for this example and is represented as (a) a straight line, (b) dots or (c) a dot and a cross.

Lewis structures also allow you to distinguish between bonding electrons and non-bonding electrons. A chlorine molecule has one pair of **bonding electrons**, which can be represented by a straight line between the two Cl atoms. The valence electrons that are not involved in bonding are called the **non-bonding electrons**. Each chlorine atom has six non-bonding electrons, present as three pairs of electrons. Pairs of non-bonding electrons are known as **lone pairs**.

Double covalent bonds

In a **double covalent bond**, two pairs of electrons are shared between the atoms.

The oxygen molecule, O_2, contains a double covalent bond. The condensed electron configuration of an oxygen atom is [He]$2s^2 2p^4$, which means that it has six electrons in its valence shell. Each oxygen atom requires two electrons to gain a stable valence shell octet of electrons. Therefore, when one oxygen atom bonds to another one, each atom shares two electrons.

As you can see in Figure 8.2.5, each oxygen atom in the molecule now has eight valence electrons. Four of these are bonding electrons and four are non-bonding electrons.

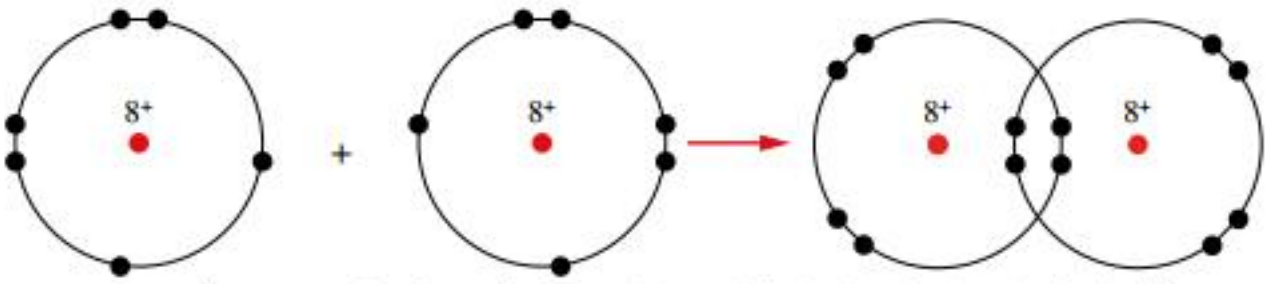


FIGURE 8.2.5 In oxygen molecules, each oxygen atom contributes two electrons to the double covalent bond between the atoms.

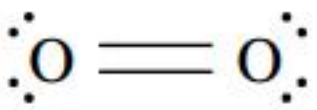


FIGURE 8.2.6 The Lewis structure shows that O_2 has a double covalent bond. Four electrons are shared and each oxygen has two lone pairs.

Figure 8.2.6 shows the Lewis structure of an oxygen molecule. The two straight lines represent two pairs of bonding electrons between the oxygen atoms, while the eight dots represent four pairs of non-bonding electrons (or four lone pairs of electrons).

Triple covalent bonds

A **triple covalent bond** occurs when three electron pairs are shared between two atoms. The nitrogen molecule, N_2, contains a triple bond. The condensed electron configuration of a nitrogen atom is [He]$2s^2 2p^3$, meaning that it has five electrons in its valence shell. A nitrogen atom requires three electrons to achieve eight electrons in its valence shell. When it bonds to another nitrogen atom, each atom contributes three electrons to the bond that forms, as shown in Figure 8.2.7. The Lewis structure of the nitrogen molecule is shown in Figure 8.2.8.

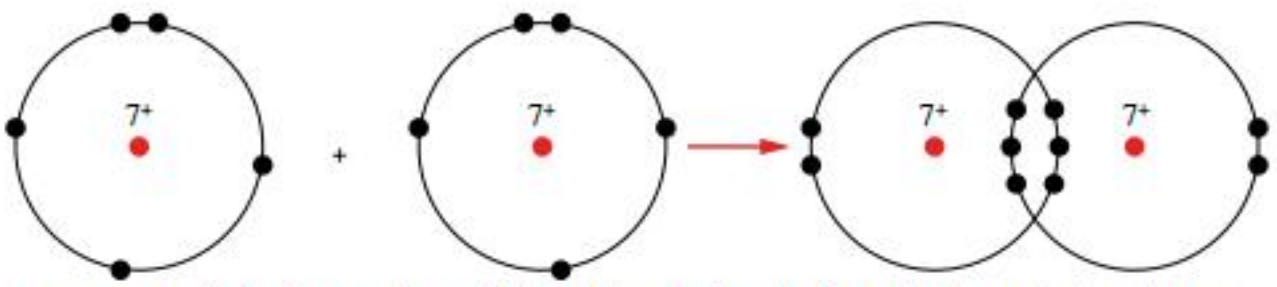


FIGURE 8.2.7 Each nitrogen atom contributes three electrons to form a triple covalent bond in a molecule of N_2.

FIGURE 8.2.8 The Lewis structure shows that N_2 has a triple covalent bond. Six electrons are shared and each nitrogen has one lone pair.

The triple covalent bond in nitrogen gas, N_2, is relatively strong and not easily broken. This means that nitrogen gas is relatively unreactive. Nitrogen is an essential element for living organisms because it is a major component of proteins and other biological molecules. Even though 78% of air is nitrogen gas, very few organisms can make use of the nitrogen because it is so unreactive. Nitrogen-fixing microorganisms are able to convert nitrogen gas into soluble nitrogen-containing compounds. These compounds are then absorbed by plants, allowing nitrogen to then be passed up the food chain.

Hydrocarbons containing single, double and triple bonds

Hydrocarbons are molecular compounds containing the elements hydrogen and carbon only. They have the general formula of C_xH_y, where the subscripts x and y represent a wide range of numerical values depending on the specific compound. Figure 8.2.9 shows the Lewis structures for three different hydrocarbons: ethane, ethene and ethyne. Each contains two carbon atoms but differs in the type of bond joining them. Ethane contains a single covalent bond between the two carbon atoms, ethene contains a double bond and ethyne contains a triple bond.

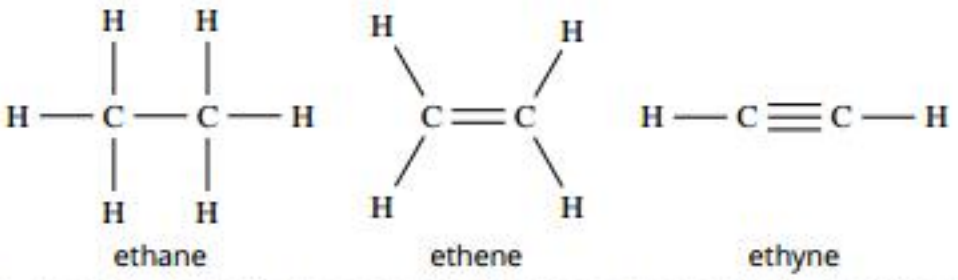


FIGURE 8.2.9 Lewis structures for three simple hydrocarbons showing single, double and triple bonds between carbon atoms

The presence of multiple bonds can greatly affect the chemical and physical properties of compounds. For example, Table 8.2.1 shows that the carbon–carbon bond lengths and bond strengths vary according to the number of bonds joining the two carbon atoms. The bond energy values in Table 8.2.1 are a measure of bond strength and you can see that the carbon–carbon triple bond is the strongest of the three; it is also the shortest. In general, triple bonds are stronger and shorter than double bonds, and double bonds are stronger and shorter than single bonds.

TABLE 8.2.1 Bond properties of hydrocarbons with single, double and triple bonds

Example of hydrocarbon	C–C bond type	C–C bond energy ($kJ\,mol^{-1}$)	Bond length (pm)
ethane	single	346	154
ethene	double	602	134
ethyne	triple	835	120

Benzene (C_6H_6) is another important hydrocarbon containing multiple bonds. The Lewis structure for benzene is often represented as a cyclic hexagon structure with alternating single and double bonds between the six carbon atoms that form a ring at the centre (Figure 8.2.10a). This structure suggests that the carbon–carbon bond lengths in benzene are different, with the single bonds being longer (~154 pm) than the double bonds (~134 pm).

However, spectroscopic analysis confirms that all C–C bond lengths in benzene are equivalent and have a length of ~140 pm, between that of a double bond and a single bond. A better representation of benzene is shown in Figure 8.2.10b. It shows that the six electrons associated with the three double bonds are spread (or delocalised) across the entire cyclic structure, making each C–C bond equal in both length and strength, and a hybrid between a single and double bond.

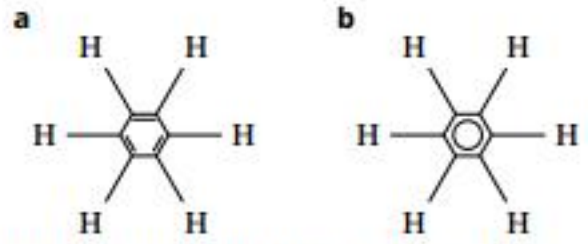


FIGURE 8.2.10 Two different representations of the benzene molecule with its six-carbon cyclic structure: (a) alternating single and double bonds and (b) the pairs of bonding electrons spread (or delocalised) across the entire cyclic structure.

FIGURE 8.2.11 Lewis structures of a hydrogen and a chlorine atom (on the left) combining to form the HCl molecule. HCl has a single covalent bond. Two electrons are shared and the Cl atom has three lone pairs.

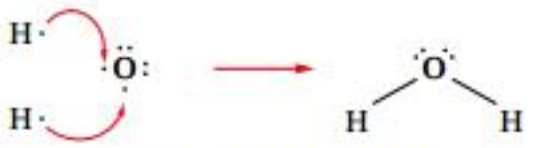


FIGURE 8.2.12 Lewis structures of two hydrogen atoms and an oxygen atom (on the left) combining to form the H_2O molecule. H_2O has two single covalent bonds. Two electrons are shared and the O atom has two lone pairs.

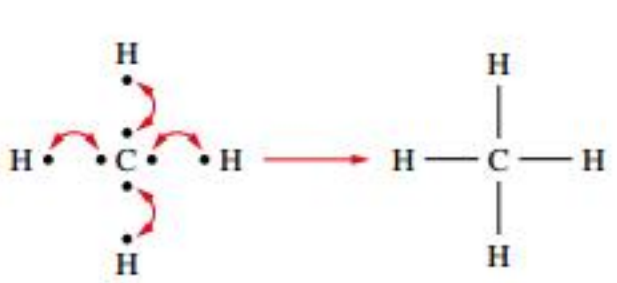


FIGURE 8.2.13 Lewis structures of four hydrogen atoms and a carbon atom (on the left) combining to form the CH_4 molecule. CH_4 has four single covalent bonds. All eight electrons are shared and there are no lone pairs.

DRAWING LEWIS STRUCTURES FOR MOLECULAR COMPOUNDS

A diatomic molecule contains two atoms. The diatomic molecules discussed so far have been elements, i.e. H_2, Cl_2, O_2 and N_2. Being elements, these molecules contain only one type of atom.

Covalent bonds can also form between atoms of different elements, producing molecular compounds. Hydrogen chloride (HCl) is a simple example (Figure 8.2.11). A hydrogen atom requires one electron to gain a stable valence shell, as does a chlorine atom. They can share an electron each to form a single covalent bond.

Polyatomic molecules

Molecules that are made up of more than two atoms are called **polyatomic molecules**. Two examples of polyatomic molecules are water and methane.

Water

When a compound forms between hydrogen and oxygen, an oxygen atom bonds with two hydrogen atoms. The oxygen atom shares one electron with each hydrogen atom. Each hydrogen atom shares one electron with the oxygen atom.

As you can see in Figure 8.2.12, a water molecule contains:

- two single covalent bonds, each containing a shared electron pair (i.e. a total of two bonding pairs of electrons)
- four non-bonding electrons on the oxygen atom (i.e. two lone pairs).

Methane

When a compound forms between carbon and hydrogen, four hydrogen atoms are needed to provide the four electrons required to have eight electrons in the valence shell of a carbon atom (Figure 8.2.13). The molecule formed is called methane and has a molecular formula of CH_4. A methane molecule has four bonding pairs of electrons and zero lone pairs.

Steps for drawing Lewis structures

The Lewis structures for HCl, H_2O and CH_4 (Figures 8.2.11, 8.2.12 and 8.2.13) are relatively straightforward examples. When drawing Lewis structures of more complex polyatomic molecules and ions the following steps provide a useful guide.

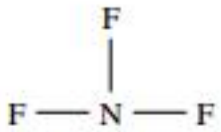
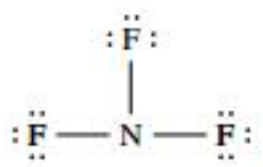
1 Sum the valence electrons from all atoms shown in the molecular formula.
   a For polyatomic anions, add the value of the negative charge to this total.
   b For polyatomic cations, subtract the value of the positive charge from this total.
2 Write atomic symbols for atoms involved to show which atoms are connected to which.
   a You must define a central atom. The central atom is typically the least electronegative (or most electropositive) atom. Electronegativity values are included in Appendix C on page 518. An easy way to determine the central atom is to find the element furthest to the left and lowest in the periodic table. Also note that hydrogen will never be a central atom in a polyatomic molecule or ion.
   b Connect the atoms using a single line representing a single pair of bonding electrons (i.e. a single bond).
   c If the molecule contains double or triple bonds you will address this in rule 5.
3 Complete octets for all peripheral atoms bonded to the central atom.
   a You do this by adding three pairs of electrons to the atomic symbol of the peripheral atom, thus giving each atom a total of eight electrons (including the two represented by the single bond).
   b The exception here is hydrogen, which can only accommodate two electrons in its valence shell—for the H atom you must think in terms of a duet rather than an octet.

4 Place any remaining electrons on the central atom.
You do this even if it gives the central atom more than an octet.
5 If there are not enough electrons to give the central atom an octet, form multiple bonds.
You do this by using one or more lone pairs from the peripheral atoms (choosing the least electronegative, or most electropositive atom).

Electronegativity is a measure of an atom's ability to attract valence electrons to itself within a chemical bond.

Worked example 8.2.1

DRAWING LEWIS STRUCTURES FOR POLYATOMIC MOLECULES

Draw the Lewis structure for nitrogen trifluoride (NF_3).	
Thinking	**Working**
Step 1: Sum the valence electrons from all atoms shown in the molecular formula.	N has the condensed electron configuration of [He]$2s^2 2p^3$, and so has five valence electrons. F has the condensed electron configuration of [He]$2s^2 2p^5$, and so has seven valence electrons. Sum of all valence electrons in $NF_3 = 5 + (3 \times 7) = 26$
Step 2: Write atomic symbols for all atoms to show which atoms are connected to which. The central atom is typically the least electronegative.	In this case, N is the least electronegative and the central atom; the three F atoms will be peripheral atoms.  A total of six electrons have been used so far, representing the three pairs of bonding electrons in the three single bonds.
Step 3: Complete octets for all peripheral atoms bonded to the central atom.	Do this by adding three pairs of electrons to the atomic symbol of the peripheral atoms.  A total of 24 electrons have been used in total so far; three bonding pairs on the central N atom and nine lone pairs across the three F atoms.
Step 4: Place any remaining electrons on the central atom.	 So far, 24 of the available 26 valence electrons have been used. There are two remaining electrons that need to be placed on the central N atom.
Step 5: If there are not enough electrons to give the central atom an octet, form multiple bonds.	 This step is not required since the central atom has a total of eight electrons surrounding it; three bonding pairs and one lone pair. The Lewis structure is complete.

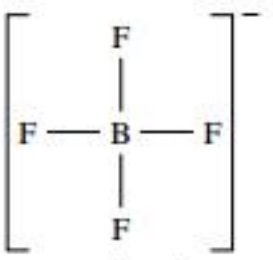
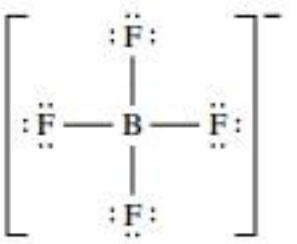
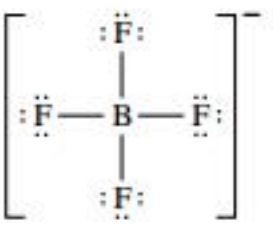
➤ Try yourself 8.2.1

DRAWING LEWIS STRUCTURE FOR POLYATOMIC MOLECULES

Draw the Lewis structure for ammonia (NH_3).

Worked example 8.2.2

DRAWING LEWIS STRUCTURES FOR POLYATOMIC IONS

Draw the Lewis structure for the boron tetrafluoride ion (BF_4^-).	
Thinking	**Working**
Step 1: Sum the valence electrons from all atoms shown in the formula.	B has the condensed electron configuration of [He]$2s^2 2p^1$, and so has three valence electrons. F has the condensed electron configuration of [He]$2s^2 2p^5$, and so has seven valence electrons. Note, in this case, the ion has a charge of 1–. Therefore, add one valence electron to the total. Sum of all valence electrons in BF_4^- = 3 + (4 × 7) + 1 = 32
Step 2: Write atomic symbols for all atoms to show which atoms are connected to which. The central atom is typically the least electronegative.	In this case, B is the least electronegative and the central atom; the four F atoms will be peripheral atoms. For polyatomic ions, put square brackets around the structure and write the charge of the ion at the top right of the brackets.  A total of eight electrons have been used so far, representing the four pairs of bonding electrons in the four single bonds.
Step 3: Complete octets for all peripheral atoms bonded to the central atom.	Do this by adding three pairs of electrons to the atomic symbol of the peripheral atoms.  A total of 32 electrons have been used in total so far; four bonding pairs on the central B atom and 12 lone pairs across the four F atoms.
Step 4: Place any remaining electrons on the central atom.	This step is not required since all 32 valence electrons have been used.  The Lewis structure is complete.
Step 5: If there are not enough electrons to give the central atom an octet, form multiple bonds.	This step is not required since the central atom has a total of eight electrons surrounding it; four bonding pairs.

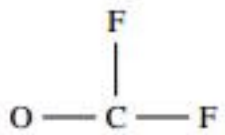
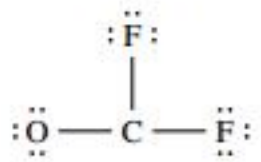
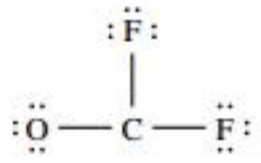
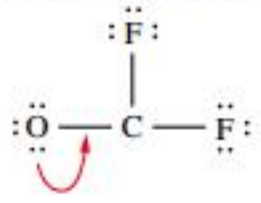
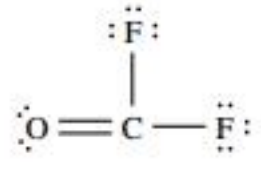
➤ Try yourself 8.2.2

DRAWING LEWIS STRUCTURES FOR POLYATOMIC IONS

Draw the Lewis structure for the ammonium ion (NH_4^+).

Worked example 8.2.3

DRAWING LEWIS STRUCTURES FOR POLYATOMIC MOLECULES WITH MULTIPLE BONDS

Draw the Lewis structure for carbonyl fluoride (COF_2).	
Thinking	**Working**
Step 1: Sum the valence electrons from all atoms shown in the molecular formula.	C has the condensed electron configuration of [He]$2s^2 2p^2$, and so has four valence electrons. O has the condensed electron configuration of [He]$2s^2 2p^4$, and so has six valence electrons. F has the condensed electron configuration of [He]$2s^2 2p^5$, and so has seven valence electrons. Sum of all valence electrons in $COF_2 = 4 + 6 + (2 \times 7) = 24$
Step 2: Write atomic symbols for all atoms to show which atoms are connected to which. The central atom is typically the least electronegative.	In this case, C is the least electronegative and the central atom; the O atom and the two F atoms will be peripheral atoms.  A total of six electrons have been used so far, representing the three pairs of bonding electrons in the three single bonds.
Step 3: Complete octets for all peripheral atoms bonded to the central atom.	Do this by adding three pairs of electrons to the atomic symbol of the peripheral atoms.  A total of 24 electrons have been used in total so far; three bonding pairs on the central C atom, three lone pairs on the O atom, and six lone pairs across the two F atoms.
Step 4: Place any remaining electrons on the central atom.	There are no remaining electrons. All of the 24 available valence electrons have been used. 
Step 5: If there are not enough electrons to give the central atom an octet, form multiple bonds.	The central C atom has only six electrons around it. Therefore, form one multiple bond (i.e. a double bond) by using a lone pair of electrons from one of the peripheral atoms. The atom chosen must be the least electronegative, which, in this case, is the O atom. Use a lone pair of electrons from the O atom to create a double bond between the C and O atoms, giving all atoms in the structure an octet.   The Lewis structure is now complete.

➤ Try yourself 8.2.3

DRAWING LEWIS STRUCTURES FOR POLYATOMIC MOLECULES WITH MULTIPLE BONDS

Draw the Lewis structure for hydrogen cyanide (HCN).

8.2 Review

SUMMARY

- The atoms in covalent molecules are held together by covalent bonds.
- A covalent bond involves the sharing of electrons.
- Covalent bonds form between non-metallic atoms, often enabling the atoms to gain valence shells containing eight electrons (except hydrogen, which gains a valence shell containing two electrons).
- A single covalent bond forms when two atoms share a pair of electrons.
- A double covalent bond forms when two atoms share four electrons (two pairs).
- A triple covalent bond forms when two atoms share six electrons (three pairs).
- Pairs of valence electrons that are not involved in bonding are called lone pairs.
- Lewis structures show the valence electron arrangements of atoms in a molecule and can be used to readily identify the number of bonding pairs and lone pairs of electrons in a molecule.

KEY QUESTIONS

Describe

1 Recall the octet rule.

2 Describe a covalent bond.

3 State the difference between a single, double and triple covalent bond.

4 List ethane, ethene and ethyne in order of:
- **a** increasing carbon–carbon bond length
- **b** increasing carbon–carbon bond strength

5 State why hydrogen is an exception to the octet rule.

Apply

6 Determine the number of covalent bonds formed between atoms in these diatomic molecules.
- **a** H_2
- **b** N_2
- **c** O_2
- **d** F_2

7 Determine the maximum number of covalent bonds an atom of each of the following elements can form.
- **a** F
- **b** O
- **c** N
- **d** C
- **e** H
- **f** Ne

8 Represent each of the following molecules using Lewis structures.
- **a** fluorine (F_2)
- **b** hydrogen fluoride (HF)
- **c** water (H_2O)
- **d** tetrachloromethane (CCl_4)
- **e** phosphine (PH_3)
- **f** carbon dioxide (CO_2)

Analyse

9 Identify the number of bonding pairs and lone pairs of electrons surrounding the central atom in the following molecules and ions.
- **a** PCl_3
- **b** BH_4^-
- **c** NI_3
- **d** H_2S
- **e** CCl_4

10 When oxygen forms covalent molecular compounds with other non-metals, the Lewis structures of these compounds typically show each oxygen atom with two lone pairs of electrons. Explain why there are two lone pairs.

11 Predict the most likely formula of the compound formed between the following pairs of elements.
- **a** N, Br
- **b** C, S

12 Represent each of the following molecules or ions using Lewis structures.
- **a** CH_3Cl
- **b** HI
- **c** H_3O^+
- **d** OH^-

13 Atom X has the condensed electron configuration of $[He]2s^22p^4$. Atom Y has the condensed electron configuration of $[He]2s^22p^5$. Deduce the likely molecular formula of the compound that will form between X and Y.

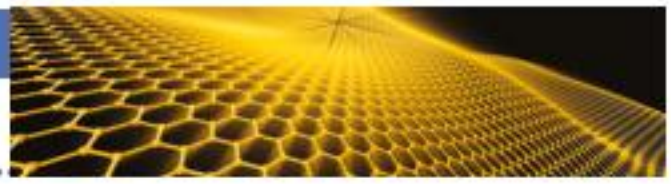
14 Compare and contrast the bonding of the oxygen atom in water (H_2O) and in methanal (CH_2O).

15 Explain why two atoms of fluorine can form a covalent bond, but two atoms of sodium are unlikely to form a covalent bond.

8.3 Naming binary molecular compounds

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- use the steps outlined to name a binary molecular compound.



A **binary molecular compound** is a compound that is made up of atoms from only two types of non-metallic elements. The previous module gave some examples of binary molecular compounds, including hydrogen chloride (HCl), water (H_2O) and nitrogen trifluoride (NF_3). Chemists need a standard way of naming these compounds. This module introduces the IUPAC naming system.

The IUPAC name of a binary molecular compound tells you which elements are in the compound, and how many atoms of each element are in one molecule.

ORDER OF ELEMENTS IN THE NAME

The element of a binary molecular compound that is named and written first is typically the one that is the least electronegative (or most electropositive). Electronegativity values are included in Appendix C on page 518. To determine which element is named first, identify which of the two elements is most to the left and lowest in the periodic table. The other element is named last and has the ending of its name changed to end in '-ide'.

For example, for a binary molecular compound that contains fluorine and phosphorus, 'phosphorus' would be the first part of the compound name, and 'fluoride' would be the last part of the compound name.

PREFIXES

Two elements can combine in more than one way to make different binary molecular compounds. For example, nitrogen and oxygen can combine as NO, NO_2 and N_2O. Each of these compounds needs to have its own name. To indicate the number of each type of atom in a binary molecular compound, a Greek prefix is used (Table 8.3.1).

TABLE 8.3.1 The Greek prefixes used to indicate the number of each type of atom

Number	Greek prefix	Number	Greek prefix
1	mono	6	hexa
2	di	7	hepta
3	tri	8	octa
4	tetra	9	nona
5	penta	10	deca

There are a couple of things to take note of when using Greek prefixes in names.

1 The 'mono' prefix is not added to the name of the first element if there is only one atom of it in the molecular formula. For example, the name of the binary molecular compound with the molecular formula PF_3 is phosphorus trifluoride, not monophosporus trifluoride.

2 If there is only one oxygen atom in the molecular formula, this is named monoxide, not monooxide. For example, the name of the compound with the molecular formula CO is carbon monoxide (not carbon monooxide), whereas the name of the compound with the formula CO_2 is carbon dioxide.

Worked example 8.3.1

NAMING BINARY MOLECULAR COMPOUNDS

Identify the name of the binary molecular compound that has the molecular formula P_2O_5.	
Thinking	**Working**
The first named element is the one that is least electronegative. This is easily determined by finding the element most to the left and lowest in the periodic table.	Phosphorus is in period 3 and group 15. Oxygen is in period 2 and group 16. The first named element is phosphorus.
The second element is then named last and has the ending of its name changed to end in '-ide'.	The second named element is oxide.
Use the Greek prefixes to indicate the number of each type of atom in the name.	There are two phosphorus atoms, so the name is diphosphorus. There are five oxygen atoms, so the name is pentaoxide. The name of P_2O_5 is diphosphorus pentaoxide.

➤ Try yourself 8.3.1

NAMING BINARY MOLECULAR COMPOUNDS

Identify the name of the binary molecular compound that has the molecular formula N_2O_4.

Binary molecular compounds containing hydrogen

For binary molecular compounds containing hydrogen, particularly those containing only one atom of the other element, Greek prefixes are not typically used to indicate the number of each type of atom based on the molecular formula. For example, H_2S is named hydrogen sulfide instead of dihydrogen monosulfide.

Common names

There are many binary molecular compounds that are officially known by their common (or trivial) names. Common names are names that do not follow a naming system. Many of these compounds are well known and have kept their historically given names. You should be able to instantly recognise that the name for H_2O is 'water'. Some more examples of common names are shown in Table 8.3.2.

TABLE 8.3.2 Some examples of common names of binary molecular compounds

Formula	Common name
H_2O	water
NH_3	ammonia
H_2O_2	hydrogen peroxide
PH_3	phosphine
N_2H_4	hydrazine

The previous module also described binary molecular compounds containing carbon and hydrogen such as ethane (C_2H_6), ethene (C_2H_4) and benzene (C_6H_6). These compounds belong to a much larger group of compounds called organic compounds. You will learn about naming organic compounds in Unit 4.

8.3 Review

SUMMARY

- A binary molecular compound is a compound that is made up of atoms from only two types of non-metallic elements.
- The first named element is the least electronegative of the two elements in the compound. This can be determined by finding the element most to the left and lowest in the periodic table.
- The other element is named last and has the ending of its name changed to end in '-ide'.
- Greek prefixes are used to indicate the number of each type of atom in the binary molecular compound.
- Many well-known binary molecular compounds are typically known by their common names. For example, H_2O is called water.

KEY QUESTIONS

Describe

1 Define a 'binary molecular compound'.

2 Describe the change to the name of the second element in the name of a binary molecular compound.

3 What number does each of these Greek prefixes refer to?

a di
b hexa
c penta
d tetra

Apply

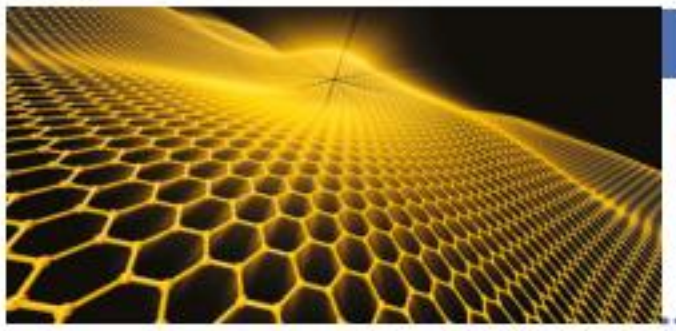
4 Name the following binary molecular compounds.

a N_2O
b CCl_4
c SF_6
d HBr
e P_4O_{10}

5 Write the molecular formulas for the following binary molecular compounds.

a phosphorus trichloride
b carbon disulfide
c dinitrogen trioxide
d dichlorine monoxide
e phosphine

8.4 Carbon networks and allotropes of carbon



BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- identify the different allotropes of carbon
- describe the different bonding structures in different allotropes of carbon
- explain the different physical and chemical properties of the allotropes of carbon in relation to their different bonding structures.

In the previous modules, you were introduced to covalent bonding in the context of substances made up of molecules. Alternatively, covalent bonding can also occur between non-metal atoms in a way that results in a continuous three-dimensional **giant covalent network** (or lattice) structure. This module will focus on two key examples of substances with a giant covalent network structure—diamond and graphite.

ALLOTROPES OF CARBON

Some elements can exist with their atoms in several different structural arrangements, called **allotropes**, which give them different physical forms. In different allotropes, the atoms are bonded to each other in different, specific ways. This gives them significantly different properties from other allotropes of the same element. Oxygen and carbon are two common elements that have different allotropic forms.

Oxygen has two allotropes. Oxygen gas consists of diatomic molecules with the formula O_2. Each oxygen atom in this arrangement is bound to one other oxygen atom. Ozone is another molecule containing only oxygen atoms. Ozone molecules have the formula O_3 and consist of a central oxygen atom bound to two other oxygen atoms. Figure 8.4.1 shows the structure of these two molecules.

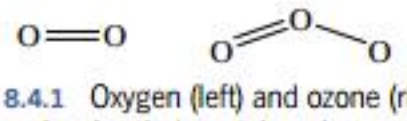


FIGURE 8.4.1 Oxygen (left) and ozone (right) are two molecules that contain only oxygen atoms.

Allotropes are different forms of the same element in which the atoms combine in different ways.

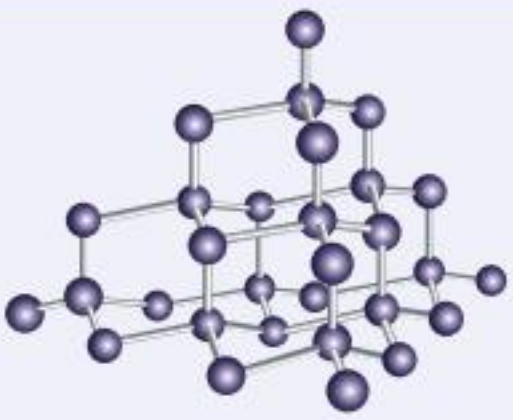
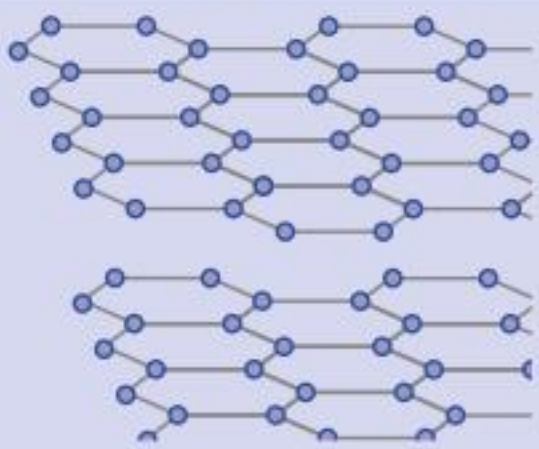
Diamonds (Figure 8.4.2) are prized for their beauty, but it is unlikely that graphite (Figure 8.4.3) will ever be held in the same esteem. Both of these minerals are made of the same single element—carbon.

FIGURE 8.4.2 Diamond is the hardest naturally occurring substance.

FIGURE 8.4.3 Natural graphite is soft and black.

Table 8.4.1 on page 165 summarises some information about the structure, properties and uses of the two most common allotropes of carbon—diamond and graphite.

TABLE 8.4.1 Comparison of properties of some of the allotropes of carbon

Allotrope	Structure	Properties	Uses
diamond	 covalent network lattice; each carbon bonded to four other carbon atoms in a tetrahedral arrangement	• very hard • sublimes (transitions directly from solid to gas) • non-conductive • brittle	• jewellery • cutting tools • drills
graphite	 covalent layer lattice; each carbon bonded to three other carbons, one delocalised electron per carbon atom	• conductive • slippery • soft • greasy	• lubricant • pencils • electrodes • reinforcing fibres

Diamond

Diamond is the hardest naturally occurring substance known.

Diamond does not contain small, discrete (individual) molecules. Instead, the carbon atoms bond to each other to form a continuous three-dimensional structure called a **covalent network lattice**. There are no weak intermolecular forces present, only strong covalent bonds. This is what gives diamond its strength.

In general, substances that have a network lattice structure have very high melting points or decomposition temperatures. They are also very hard because the atoms are held firmly in fixed positions in the lattice.

As you will see in Chapter 11, when an atom has four electron pairs in its valence shell, the electron pairs position themselves as far away from each other as possible in a **tetrahedral shape**. In the covalent network lattice for diamond shown in Figure 8.4.4, you can also see that individual atoms within diamond form single covalent bonds to four other carbon atoms in a tetrahedral arrangement.

The properties of diamond are directly related to its structure.

- Single covalent bonds between carbon atoms are strong bonds. The entire structure of a diamond consists of a continuous network of these bonds, making diamond very hard and rigid.
- There are no molecules of diamond. There are only strong covalent bonds between carbon atoms, which makes the **sublimation** point of diamond very high, at around 3500°C—sublimation is the process of transitioning from the solid state to the gaseous state without passing through the liquid state.
- The rigidity means that diamonds are brittle and break rather than bend.
- Diamond does not conduct electricity because it does not contain any charged particles that are free to move.

i Diamond is made up of carbon atoms that bond with four neighbouring carbon atoms, forming a covalent network lattice. This structure makes diamond extremely hard.

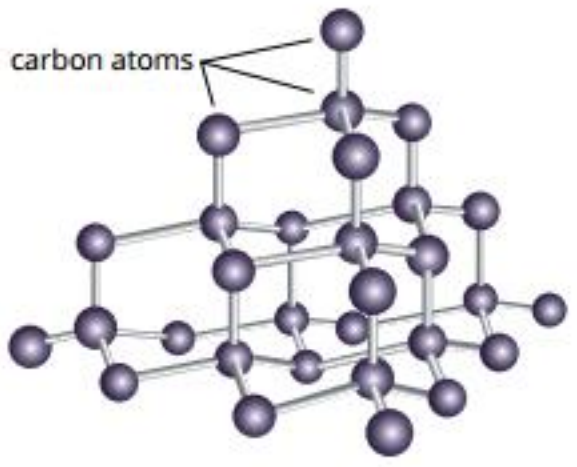


FIGURE 8.4.4 The structure of diamond showing each carbon atom with four single covalent bonds to neighbouring atoms

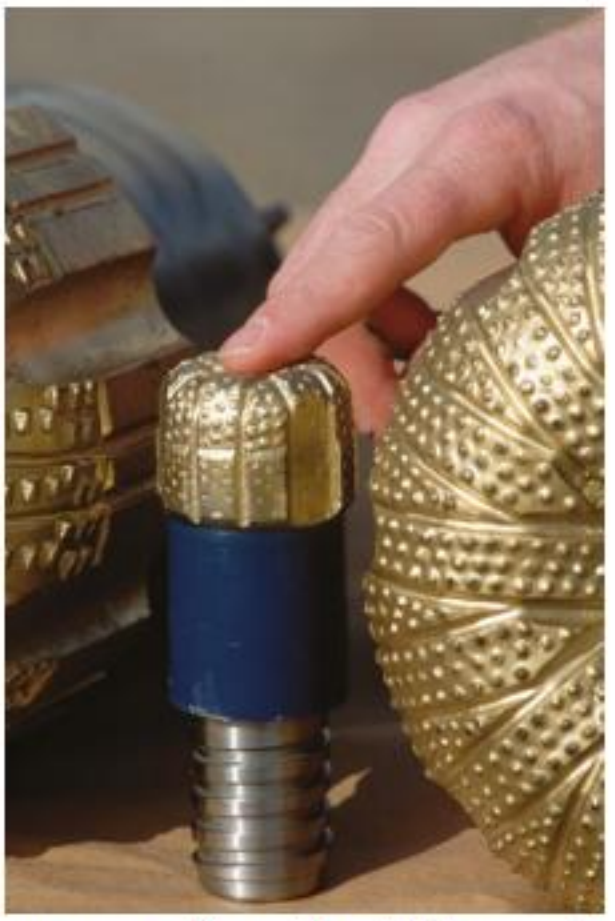


FIGURE 8.4.5 Diamond-tipped drills are used to drill through rock in the fracking industry.

- Because the atoms in diamonds are held together very strongly, the thermal conductivity is extremely high. It is five times greater than that of copper, leading to some specialty electronic uses where diamond is used to transfer heat away from some important electrical components.

The crystalline appearance of diamonds and their high refractive index (bending of light) make them sparkle and have made them extremely popular as jewellery, but the hardness of diamond also lends itself to industrial uses. Many industrial cutting and drilling tools for working with tough materials are diamond-tipped. The drill tips in Figure 8.4.5 are used to drill through rock in the fracking industry. They contain small pieces of diamond that improve the hardness and durability of the tool.

Graphite

Graphite is a very different form of carbon. As you can see in Figure 8.4.6, the carbon atoms in **graphite** are in layers. The atoms are arranged in a series of interlocking hexagonal shapes in a two-dimensional layer, and these layers are then arranged in stacks. There are strong covalent bonds between the carbon atoms in each layer. However, there are weak intermolecular forces between the layers. As a consequence, it is hard in one direction but quite slippery and soft in another direction. The structure of graphite is referred to as a **covalent layer lattice**.

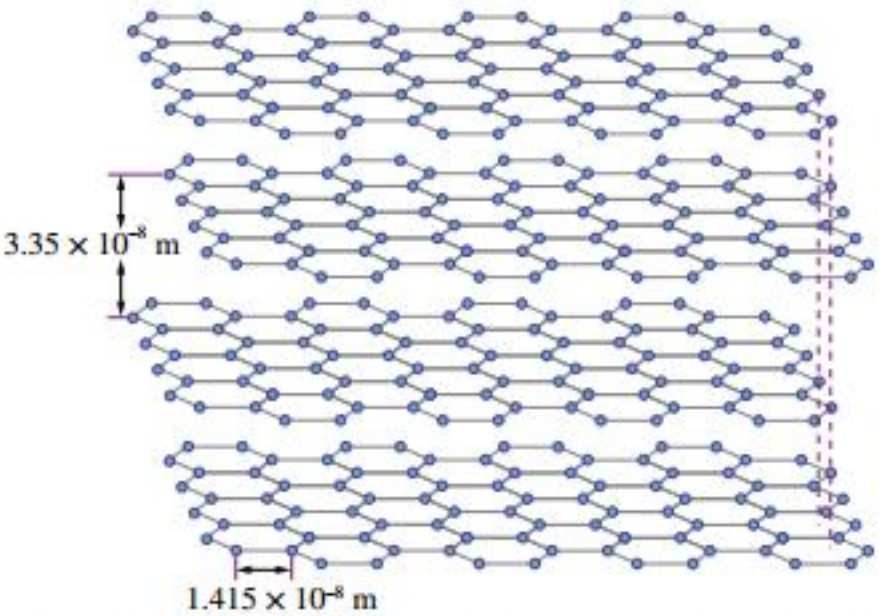


FIGURE 8.4.6 Graphite has a covalent layer lattice structure. The carbon atoms within each layer are covalently bonded to each other. Weak intermolecular forces exist between the layers.

The covalent layer lattice structure of graphite also explains some of its other properties.

- The strong covalent bonds between the atoms in each layer explain graphite's resistance to heat. Graphite sublimes at a temperature of about 3600°C.
- Each carbon atom is bonded to three other carbon atoms. The fourth valence electron from each atom is able to move within the layer. The electrical conductivity of graphite is due to these delocalised electrons.

The conductivity of graphite makes it suitable for applications such as battery electrodes, where conductivity is required but a metal is not suitable.

Graphite can also be used as a lubricant. The weak intermolecular forces between layers allow these layers to slide over each other and to reduce the friction between moving parts, such as in locks or machinery, as shown in Figure 8.4.7 on page 167.

Graphite is also used as an additive to improve the properties of rubber products and it can be woven into a fibre. This helps to reinforce plastics. Spun graphite fibre can be used to make strong composite materials such as those used in tennis racquets, fishing rods and racing car shells.

In graphite, each carbon atom is covalently bonded to three other carbon atoms. The layered network structure contains delocalised electrons. Bonds within the layers are strong, but the attractive forces between layers are weak intermolecular forces.

FIGURE 8.4.7 Graphite lubricant helps machinery run smoothly.

Fullerenes

In the late 1970s, while working at the Australian National University in Canberra, Dr Bill Burch discovered a new allotrope of carbon. This allotrope was made up of molecules containing a roughly spherical group of carbon atoms arranged in a series of pentagons and hexagons, similar to the shape of a soccer ball, as you can see in Figure 8.4.8.

FIGURE 8.4.8 The structure of a fullerene has a similar pattern to the surface of some soccer balls.

> **Fullerenes are an allotrope of carbon where the atoms are arranged in a series of pentagons and hexagons.**

These molecules have similar structures to the geodesic (curved surface) designs of architect Richard Buckminster 'Bucky' Fuller and scientists have found variations of these molecules in other shapes. The molecules are called **fullerenes**, although they are more commonly referred to as **buckyballs**. Figure 8.4.9 shows the Biosphere in Montreal, Canada—a museum designed by Buckminster Fuller.

Fullerenes have three covalent bonds to each carbon atom and in some ways appear to be similar to graphite. This leaves delocalised electrons in the structure and the possibility of electrical conductivity. Although fullerenes were initially just a curiosity, scientists predict that they have significant potential in a number of fields such as composite materials and photovoltaic cells (solar panels). The most stable fullerene molecule involves 60 carbon atoms bonded into an approximately spherical shape that is known as buckminsterfullerene or C_{60}.

FIGURE 8.4.9 The Biosphere in Montreal, Canada, is a museum designed by Buckminster Fuller.

Graphene

You have seen that graphite has a layered structure. **Graphene** is best described as a single layer of graphite (Figure 8.4.10 on page 168). Graphene is a single-layer sheet with the same arrangement as the layers stacked in graphite—each carbon atom is bonded to three other carbon atoms arranged in a series of interlocking hexagonal shapes, forming a two-dimensional layer or sheet. It is a relatively new material and was first isolated in 2004.

FIGURE 8.4.10 Graphene is a single-layer sheet with the same arrangement as the layers that are stacked in graphite.

Graphite is soft due to the weak intermolecular forces between its layers. Graphene, being only a single layer, retains the electrical conductivity of graphite but is an extremely strong and tough material.

Graphene has many potential uses. Graphene could:

- replace silicon as the basis for computer chips and circuits due to its high electrical conductivity
- be used in desalination plants; water under pressure can pass through the thin layer, but dissolved impurities cannot
- be used to construct electrodes, where it is an advantage for an electrode to be a non-metal
- be used in organic photovoltaic cells
- be used to reinforce composite materials because of its strength.

An interesting feature of graphene is that, because it is a single layer, every carbon atom is available for reaction from two sides at any instant during a chemical reaction.

Carbon nanotubes

Nanotubes are closely related to graphene. They are called nanotubes because they have a long, hollow structure with walls formed from graphene. The diameter of these cylinders is very small, around 1 nanometre (10^{-9} metre) wide, while they can be millions of times longer. They can be capped on the end of each cylinder by half a fullerene molecule as shown in Figure 8.4.11.

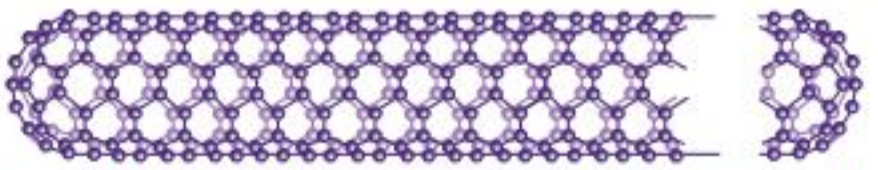


FIGURE 8.4.11 A carbon nanotube can be regarded as a sheet of graphene rolled into a cylinder and capped on the ends by half a fullerene molecule.

Nanotubes can be single-walled or multi-walled. A multi-walled nanotube has smaller tubes sitting inside larger tubes.

Scientists are interested in nanotubes because of their:

- unique strength
- electrical conductivity (the conductivity of nanotubes depends on their shape; some are conductors and others are semiconductors)
- thermal conductivity
- strong forces of attraction to each other.

Nanotubes hold great promise in fields such as optics, nanotechnology and electronics. Their extraordinary strength and thermal and electrical conductivity suggest they may be useful as additives in various structural materials.

8.4 Review

SUMMARY

- Allotropes are different forms of the same element in which the atoms combine in different ways.
- The two most common allotropes of carbon are diamond and graphite. The structures and properties of these allotropes are very different.
- In diamond, each carbon atom is covalently bonded to another four carbon atoms in a tetrahedral shape, forming a covalent network lattice structure. Diamond sublimes at a high temperature, is extremely hard and has a sparkling, crystalline appearance.
- In graphite, each carbon atom is covalently bonded to three other carbon atoms. The layered network structure contains delocalised electrons. Bonds within the layers are strong, but bonds between layers are weak intermolecular forces. Graphite is slippery, conducts electricity and sublimes at a high temperature.
- Since the late 1970s, scientists have developed a range of new carbon allotropes such as fullerenes, graphene and carbon nanotubes.
- These carbon allotropes are of interest to scientists because of their enhanced properties such as their high tensile strength and high electrical and thermal conductivity.

KEY QUESTIONS

Describe

1 State what is unusual about the electrical conductivity of graphite given that carbon is a non-metal.

2 State the number of covalent bonds formed by each carbon atom in diamond and in graphite.

3 Classify the following as either a use of diamond or a use of graphite: jewellery, composite materials, electrodes, pencil lead, industrial saw blades, lubricants, drill bits, heat conductor.

Apply

4 Identify a physical property that diamond and graphite have in common.

5 **a** Explain what is meant by the word 'sublime'.
b Explain why diamond and graphite only sublime at temperatures over 3500°C.

6 Explain the following properties of diamond in terms of its bonding and structure.
a hardness or softness
b ability or inability to conduct electricity
c ability or inability to conduct heat

7 Explain the following properties of graphite in terms of its bonding and structure.
a hardness or softness
b ability or inability to conduct electricity

8 Describe the bonding within a C_{60} buckyball.

Analyse

9 Compare and contrast the structures and properties of fullerenes and graphite.

10 Differentiate between graphene and graphite.

Chapter review

08

KEY TERMS

allotrope
binary molecular compound
bonding electron
buckyball
covalent bond
covalent compound
covalent layer lattice
covalent network lattice
diamond
diatomic molecule
double covalent bond
electron dot diagram
fullerene
giant covalent network
graphene
graphite
intermolecular force
intramolecular bond
Lewis structure
lone pair
molecular compound
molecular element
molecular formula
molecule
nanotube
non-bonding electron
octet rule
polyatomic molecule
single covalent bond
sublimation
tetrahedral shape
triple covalent bond

KEY QUESTIONS

Describe

1 Which one of the following statements is the best description of a molecule?
- **A** A molecule is a compound formed by an electron transfer between two non-metal atoms.
- **B** A molecule is a discrete group of covalently bonded atoms.
- **C** A molecule is a compound that contains single covalent bonds.
- **D** A molecule is a compound that contains only covalent bonds.

2 Identify the statement that best describes the way hydrogen atoms bond to each other.
- **A** One hydrogen atom donates an electron to another hydrogen atom to form a molecule.
- **B** Hydrogen atoms form a lattice with delocalised electrons.
- **C** Hydrogen atoms share electrons to obtain a complete valence shell of eight electrons.
- **D** Two hydrogen atoms share an electron each to form a hydrogen molecule.

3 State how many valence electrons each of the following atoms has.
- **a** C
- **b** Se
- **c** Al
- **d** I
- **e** Si

4 Show Lewis structures for the following atoms.
- **a** nitrogen
- **b** oxygen
- **c** hydrogen
- **d** chlorine
- **e** fluorine

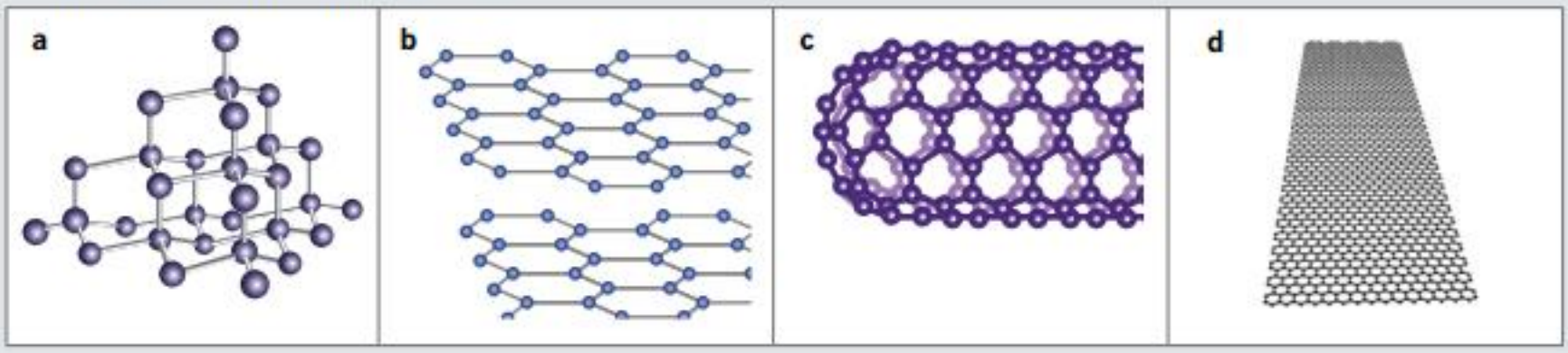
5 Show the formation of the following elemental molecules using Lewis structures.
- **a** the formation of the H_2 molecule from two H atoms
- **b** the formation of the O_2 molecule from two O atoms
- **c** the formation of the N_2 molecule from two N atoms

6 Show the formation of the following molecular compounds using Lewis structures.
- **a** the formation of the HCl molecule from an H atom and a Cl atom
- **b** the formation of the H_2O molecule from two H atoms and one O atom
- **c** the formation of the CH_4 molecule from one C atom and four H atoms

7 Indicate whether the following statements about carbon dioxide (CO_2) are true or false.
- **a** Carbon dioxide is a molecular compound.
- **b** A molecule of carbon dioxide contains three atoms.
- **c** The bonds between the carbon and oxygen atoms in carbon dioxide are intramolecular bonds.
- **d** There are two single covalent bonds in a molecule of carbon dioxide.
- **e** There are four lone pairs of electrons in a molecule of carbon dioxide.

8 Identify the nature of the carbon–carbon bonding in diamond from the following list.
- **A** The carbon–carbon bond is a double covalent bond.
- **B** The carbon–carbon bond is a triple covalent bond.
- **C** A carbon atom is covalently bonded to four other carbon atoms to form the C_5 molecule.
- **D** The carbon–carbon bond is a single covalent bond that forms the C_2 molecule.
- **E** Each carbon atom is covalently bonded to four other carbon atoms in a tetrahedral arrangement, forming a giant network lattice structure.

9 State the allotrope name, bonding feature and properties of the following structures.



Apply

10 The following substances all contain carbon atoms. Which one will have the highest boiling point (or sublimation point)?

A carbon dioxide
B methane
C graphite
D ethyne

11 Covalent substances generally do not contain free-moving charged particles. Explain what this indicates about their general physical properties.

12 Solid carbon dioxide sublimes when it is heated; that is, it goes straight from a solid to a gas. Explain what happens to the bonds in carbon dioxide when it sublimes. Use the terms 'intramolecular bonds' and 'intermolecular forces' in your answer.

13 In a molecule of nitrogen (N_2), determine how many of the following there are.

a bonding electrons
b covalent bonds
c non-bonding electrons

14 Explain why neon atoms do not form covalent bonds.

15 Draw Lewis structures for each of the following molecules and identify the number of bonding and non-bonding electrons in each molecule.

a HBr
b H_2O
c CF_4
d C_2H_6
e PF_3
f CH_4
g H_2S

16 Name the following binary covalent compounds.

a NO_2
b S_2F_2
c PCl_5
d H_2O_2

17 Explain why graphite sublimes at a high temperature, conducts electricity and can be used as a lubricant.

18 Draw Lewis structures for the NO^+ ion and the NO_2^- ion, and state the number of bonding and lone pairs of electrons in each ion.

19 Elements X and Y are represented by the following Lewis structures.

$$\dot{X} \qquad \cdot\ddot{Y}:$$

a If X and Y were to form a molecular compound, determine what the formula would be.
b Name three possible real compounds that this compound could be.

20 Draw Lewis structures for nitrogen (N) and fluorine (F). Use these to predict the chemical formula for the molecular compound that forms between N and F. Draw the Lewis structure of the compound to confirm your prediction.

Analyse

21 Explain why covalent molecular substances generally have lower melting and boiling points than metallic, ionic and giant covalent network substances.

22 The formula of a molecule is XY_4. Identify the alternative that could match this formula.

A OH_4
B CH_4
C HBr_4
D CO_4

23 Compare and contrast Lewis structures for neon and methane. Identify the ways in which the electron arrangements around neon and carbon are similar and in what ways are they different.

24 Differentiate between the non-metallic elements argon (Ar) and chlorine (Cl) in terms of their electron configurations and the types of bonds their atoms form with other atoms.

25 Determine how many lone pairs of electrons are in each of the following molecules and state which atom they are associated with.

a H_2
b NH_3
c HCl
d O_2

26 Identify which is the central atom in each of the following polyatomic molecules or ions. Deduce the number of bonding pairs and lone pairs of electrons that are found around the central atom in each.

a NF_3
b BF_4^-
c COF_2

27 Consider the following list of covalent molecular substances: N_2, Cl_2, O_2, NH_3, HCl, CH_4, H_2O, CO_2, CCl_4, $CHCl_3$. From the list, identify and draw the Lewis structure of the molecule that has the following features.

a one triple bond
b one double bond
c two double bonds
d two single bonds

28 Based on the molecular formula of each binary molecular compound, determine whether the stated name is correct or incorrect. If the name is incorrect, explain why, and then determine the correct name.

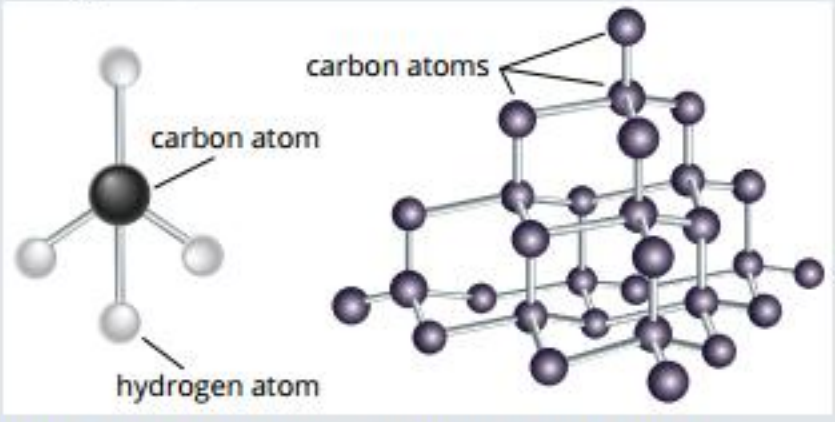
a HBr is monohydrogen monobromide
b N_2O_5 is dinitrogen pentaoxide
c C_2H_6 is hexahydrogen dicarbide
d P_4O_6 is tetraphosphate hexoxide

29 The atoms in molecules of nitrogen (N_2), oxygen (O_2) and fluorine (F_2) are held together by covalent bonds. Describe how the bonds in these molecules are:

a similar
b different.

30 Compare and contrast the carbon–carbon bonding in ethene and benzene.

31 The structures of methane and diamond are shown in the following image. Each carbon atom in methane (CH_4) has a tetrahedral arrangement of atoms around it. A carbon atom in diamond also has a tetrahedral arrangement.



a Describe all the types of bonding that would be present in each substance.
b Use the types of bonding present in each substance to explain the different properties you would expect each to have.

32 The table below lists some key properties of diamond and graphite.

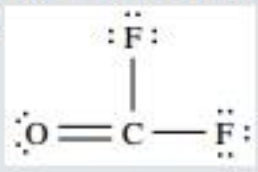
Material	Hardness (Moh scale)	Electrical conductivity ($S\,m^{-1}$)	Thermal conductivity ($W\,m^{-1}\,K^{-1}$)
diamond	10	10^{-13}	2000
graphite	<1	3×10^5	200

a Explain the difference in hardness and electrical conductivity of diamond and graphite, referring to the structure and bonding of each substance.
b When discussing the conductivity of diamond and graphite, why it is important to be specific as to what type of conductivity you are referring to?
c One method used by jewellers to test the quality of diamonds is to heat them to 1000°C and time the rate of cooling. Deduce how a high-quality diamond with few impurities would compare to a low-quality diamond in this test.

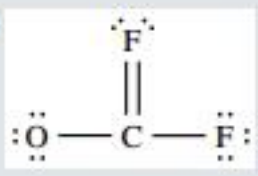
Interpret

33 Decide which of the following Lewis structures for carbonyl fluoride (COF_2) is the most appropriate and justify your decision.

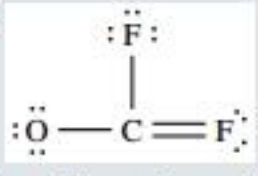
A



B



C



34 Silicon lies under carbon in the periodic table and may be expected to have similar chemical and physical properties. The compound carbon dioxide (CO_2) is a molecular compound that is a colourless gas at room temperature with a sublimation point of –78.5°C. The compound silicon dioxide (SiO_2) is a crystalline solid at room temperature with a melting point of 1710°C and a boiling point of 2230°C. Determine how you would reconcile these differences in properties between CO_2 and SiO_2.

35 Draw a possible Lewis structure for the perchlorate ion (ClO_4^-) that obeys the octet rule for all atoms. Evaluate what is unusual about the covalent bonding in the molecular ion based on your understanding of the number of covalent bonds typically formed by chlorine and oxygen atoms.

CHAPTER

09 The mole, molar mass and stoichiometry

Chemists in fields as diverse as environmental monitoring, pharmaceuticals and fuel production routinely carry out chemical reactions in their work. It is important for them to be able to measure specific quantities of chemicals quickly and easily, in part because the amount of products formed depends on the amount of reactants.

At the end of this chapter, you will have a greater understanding of the ways in which chemists measure quantities of chemicals and, in particular, how they can accurately count the number of particles in samples of elements and compounds simply by weighing them. This is essential for designing and producing materials, including cosmetics, fuels, fertilisers, pharmaceuticals and building materials.

Syllabus subject matter

Topic 3 • Chemical reactions—reactants, products and energy change

MOLE CONCEPT AND LAW OF CONSERVATION OF MASS

- State that a mole is a precisely defined quantity of matter equal to Avogadro's number of particles. **9.2**
- State the law of conservation of mass. **9.4**
- Explain that the mole concept relates mass, moles and molar mass. **9.2, 9.4**
- Apply the mole concept to calculate the mass of reactants and products; amount of substance in moles; number of representative particles; and molar mass of atoms, ions, molecules and formula units. (Formula: moles (n) = $\frac{\text{mass (m)}}{\text{molar mass (M)}}$) **9.2, 9.4**
- Determine the percentage composition from relative atomic masses; empirical formula of a compound from the percentage composition by mass; and molecular formula of a compound from its empirical formula and molar mass. **9.3**
- Determine limiting reactants. **9.4**
- Discriminate between experimental and theoretical yield. **9.4**
- Analyse data to determine percentage and theoretical yield. (Formula: percentage yield$(\%) = \frac{\text{experimental yield}}{\text{theoretical yield}} \times \frac{100}{1}$) **9.4**

CHEMICAL REACTIONS

- Determine balanced chemical equations, including state symbols (s), (l), (g) and (aq), for a variety of reactions, e.g. single displacement, double-displacement, acid–base, combustion, combination, decomposition and simple redox reactions.* **9.4**

*The greyed-out section of this dot point is addressed explicitly in another chapter.

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9.1 Atomic mass, molecular mass and formula mass

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the concepts of atomic mass and relative atomic mass
- explain how 1 atomic mass unit is equal to $\frac{1}{12}$ the mass of a carbon-12 atom
- analyse relative atomic mass data
- describe the concepts of relative molecular mass and relative formula mass
- calculate relative molecular mass and relative formula mass.

FIGURE 9.1.1 (a) A teaspoon of sucrose crystals contains an incredibly large number of extremely small sucrose molecules. (b) The single sucrose molecule pictured is made of 12 carbon atoms (black), 22 hydrogen atoms (white) and 11 oxygen atoms (red).

By now we know quite a few things about atoms, molecules and ions. We know that:

- they are very small, of the order of picometres
- their masses are also very small, of the order of 10^{-24} g for the hydrogen atom
- their numbers are huge—even very small samples of matter contain billions of trillions of atoms; for example, just one granule of table sugar can contain as many as 4.9×10^{19} atoms—that is 49 000 000 000 000 000 000 atoms!

The chemical name for table sugar is sucrose (Figure 9.1.1a). Sucrose is a type of sugar that is extracted and refined from sugarcane, which is grown in many areas of Queensland. Figure 9.1.1b shows a model of a sucrose molecule. One sucrose molecule contains 12 carbon atoms, 22 hydrogen atoms and 11 oxygen atoms bonded together, and has a total mass of 5.7×10^{-22} g—that is 0.000 000 000 000 000 000 000 57 grams.

Such small masses are not easily measured, and such large numbers are not easily counted. These very small and very large numbers can also be inconvenient to use in calculations. This module will introduce you to the ways that scientists determine the masses of atoms, molecules and ions, while in the next module you will learn how to count the very large numbers of these particles.

ATOMIC MASSES

Chemistry is a quantitative science, so knowing the mass of atoms is essential. Due to the extremely small mass of atoms, it is impossible to weigh an individual atom. What scientists can do is use **mass spectrometry** to compare the relative masses of atoms. Mass spectrometry is described in Chapter 5, beginning at page 82.

The first step in determining the relative mass of atoms is to give a value to the mass of a reference atom. This atom can then be used as a standard to compare to all other atoms. Prior to 1961, oxygen was used as the standard, but physicists and chemists could not agree on a way of assigning a standard mass to oxygen. Chemists assigned a mass of exactly 16 to the average mass of oxygen atoms. Physicists assigned a mass of exactly 16 to the oxygen-16 isotope. This resulted in two different tables of slightly different atomic masses. In 1961, by international agreement, the carbon-12 (or ^{12}C) atom was chosen as the standard atom and given an atomic mass of exactly 12 units of mass. **Atomic mass** is therefore defined as the mass of an atom in **atomic mass units (amu)**. ^{12}C is the isotope of carbon that has exactly 6 protons, 6 neutrons and 6 electrons and is assigned a mass of exactly 12 amu. Therefore, one atomic mass unit is defined as a mass exactly equal to $\frac{1}{12}$ the mass of a ^{12}C atom.

i Atomic mass is the mass of an atom in atomic mass units. One atomic mass unit (amu) is defined as a mass exactly equal to $\frac{1}{12}$ the mass of a ^{12}C atom.

Assigning ^{12}C an atomic mass of 12 amu allows other atoms to be given a mass value in amu that is relative to the mass of a ^{12}C atom. When a hydrogen-1 atom is experimentally compared to ^{12}C using a mass spectrometer, it is found on average to be 8.400% the mass of ^{12}C. If hydrogen has 8.400% the mass of ^{12}C, it would have a relative atomic mass of 1.008 (0.08400 × 12 amu = 1.008 amu).

RELATIVE ATOMIC MASS

You were introduced to the concept of relative atomic mass in Chapter 5. The periodic table at the back of the book provides relative atomic masses for each element. The value for chlorine, for example, is 35.45. Naturally occurring chlorine has two isotopes, as shown in Figure 9.1.2. The relative abundance of each isotope is listed in Table 9.1.1. In Chapter 5, you looked at how the relative atomic mass (A_r) of chlorine is calculated from this data using the formula:

$$A_r = \frac{(\text{relative isotopic mass} \times \% \text{ abundance}) + (\text{relative isotopic mass} \times \% \text{ abundance})}{100}$$

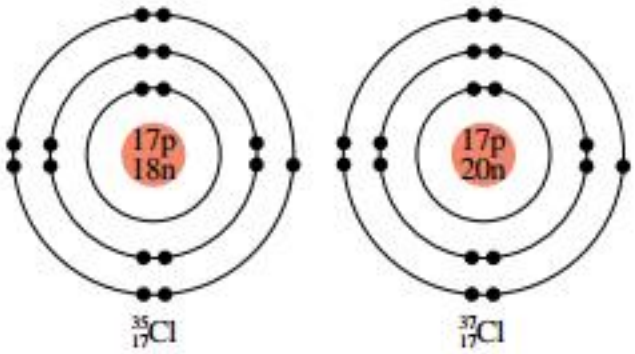


FIGURE 9.1.2 The two isotopes of the element chlorine. Different numbers of neutrons in the nuclei of these atoms give the atoms different masses.

TABLE 9.1.1 The isotopic composition of chlorine

Isotope	Relative isotopic mass	Relative abundance (%)
^{35}Cl	34.969	75.80
^{37}Cl	36.966	24.20

As you can see, the value of 35.45 is between the masses of the two chlorine isotopes but is closer to that of ^{35}Cl as it is the more abundant isotope. Other examples of relative atomic masses include the following.

- Naturally occurring magnesium consists of three isotopes and the weighted average of these isotopes gives: $A_r(Mg) = 24.31$
- Naturally occurring copper consists of two isotopes and the weighted average of these isotopes gives: $A_r(Cu) = 63.55$

Note that the relative atomic mass has no unit because it is a ratio. It compares the weighted average mass of an element to $\frac{1}{12}$ of the mass of the ^{12}C atom.

The relative atomic mass (A_r) of an element is the weighted average of the atomic masses of the isotopes of the element on the ^{12}C scale. Relative atomic mass is a dimensionless quantity with no units.

RELATIVE MOLECULAR MASS

Some elements and compounds exist as **molecules**; for example, oxygen (O_2), nitrogen (N_2) and carbon dioxide (CO_2). In Chapter 8, you learnt how non-metallic elements bond together to form covalent molecules. For these substances, a **relative molecular mass (M_r)** can be calculated by taking the sum of the relative atomic masses of all atoms in the molecular formula.

The relative molecular mass is the average mass of a molecule in a molecular compound. It is numerically equal to the sum of the relative atomic masses of all the atoms in the molecular formula.

Worked example 9.1.1

CALCULATING THE RELATIVE MOLECULAR MASS OF MOLECULES

Calculate the relative molecular mass of carbon dioxide (CO_2).	
Thinking	**Working**
Use the periodic table to find the relative atomic mass for the elements represented in the formula.	$A_r(C) = 12.01$ $A_r(O) = 16.00$
Determine the number of atoms of each element present, taking into consideration any brackets in the formula.	1 × C atom 2 × O atoms
Determine the relative molecular mass by adding the appropriate relative atomic masses.	$M_r = 1 \times A_r(C) + 2 \times A_r(O)$ $= 1 \times 12.01 + 2 \times 16.00$ $= 44.01$

➤ Try yourself 9.1.1

CALCULATING THE RELATIVE MOLECULAR MASS OF MOLECULES

Calculate the relative molecular mass of nitric acid (HNO_3).

RELATIVE FORMULA MASS

The relative formula mass is the average mass of one formula unit in an ionic compound. It is numerically equal to the sum of the relative atomic masses of all the atoms in the formula unit.

You learnt in Chapter 7 that ionic compounds, such as sodium chloride (NaCl) and magnesium oxide (MgO), do not exist as molecules but rather as ionic lattices. For ionic compounds, the term **relative formula mass** is used. Relative formula mass, like relative molecular mass, is calculated by taking the sum of the relative atomic masses of all the atoms in the formula unit.

Worked example 9.1.2

CALCULATING THE RELATIVE FORMULA MASS OF IONIC COMPOUNDS

Calculate the relative formula mass of magnesium hydroxide ($Mg(OH)_2$).

Thinking	Working
Use the periodic table to find the relative atomic mass for the elements represented in the formula.	A_r(Mg) = 24.31 A_r(O) = 16.00 A_r(H) = 1.01
Determine the number of atoms of each element present, taking into consideration any brackets in the formula.	1 × Mg atom 1 × 2 = 2 O atoms 1 × 2 = 2 H atoms
Determine the relative formula mass by adding the appropriate relative atomic masses.	relative formula mass = $1 \times A_r(Mg) + 2 \times A_r(O) + 2 \times A_r(H)$ $= 1 \times 24.31 + 2 \times 16.00 + 2 \times 1.01$ $= 58.33$

➤ Try yourself 9.1.2

CALCULATING THE RELATIVE FORMULA MASS OF IONIC COMPOUNDS

Calculate the relative formula mass of copper(II) nitrate ($Cu(NO_3)_2$).

Table 9.1.2 summarises the different types of relative mass described in this module.

TABLE 9.1.2 Relative mass terms

Relative mass term	Example	Value of relative mass
relative atomic mass	O	16.00
relative molecular mass	SO_2	32.07 + 2 × 16.00 = 64.07
relative formula mass	K_2O	2 × 39.10 + 16.00 = 94.20

9.1 Review

SUMMARY

- Atomic mass is the mass of an atom in atomic mass units (amu).
- Most elements consist of a mixture of isotopes.
- The most common isotope of carbon, carbon-12 (^{12}C), is used as the reference standard to compare the masses of atoms.
- The carbon-12 isotope is assigned a mass of exactly 12 amu.
- The relative atomic mass, A_r, of an element is a weighted average of its isotopic masses. It has no units.
- The relative molecular mass of molecules and the relative formula mass of ionic compounds are calculated from the sum of the relative atomic masses of all atoms present in the chemical formula.

KEY QUESTIONS

Describe

1 **a** State the isotope accepted as the standard for the atomic mass scale.

b What is the value (including units) of this isotope for quantifying atomic mass?

2 Describe the concept of atomic mass.

3 What makes up most of the atomic mass of an atom?

4 State the symbol for relative molecular mass.

5 Recall how relative molecular mass and relative formula mass are calculated.

Apply

6 Why does the periodic table list the relative atomic mass of carbon as 12.01 when the scale is based on ^{12}C being assigned a mass value of exactly 12?

7 The atomic mass of any atom such as a chlorine-35 atom is known. Even though this mass value is known with high accuracy and precision, it would be difficult to obtain and weigh a sample that contained one million chlorine-35 atoms. State two reasons why this might be a difficult task.

8 Explain why the ionic compound copper(II) sulfate ($CuSO_4$) does not have a relative molecular mass.

9 Explain why the relative atomic mass for chlorine, shown in Table 9.1.1 on page 175 cannot be calculated by adding the isotopic masses of the two isotopes together and dividing by two.

Analyse

10 Differentiate between atomic mass and relative atomic mass.

11 The relative atomic mass of some elements is, or is very close to being, a whole number. Fluorine is an example. The relative atomic mass of other elements such as magnesium is not close to being a whole number. Provide an explanation for why this is the case.

12 Three isotopes of potassium exist: ^{39}K, ^{40}K and ^{41}K. Given that the relative atomic mass of potassium is 39.1, which isotope is the most abundant? Give a reason for your answer.

13 Calculate the relative molecular mass of:

a sulfuric acid (H_2SO_4)

b ammonia (NH_3)

c ethane (C_2H_6)

14 Calculate the relative formula mass of:

a potassium chloride (KCl)

b sodium carbonate (Na_2CO_3)

c aluminium sulfate ($Al_2(SO_4)_3$)

15 Determine the:

a relative atomic mass of fluorine

b relative molecular mass of fluorine gas, F_2

c relative formula mass of magnesium fluoride, MgF_2

d relative molecular mass of nitronium tetrafluoroborate, NO_2BF_4

9.2 Introducing the mole

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the concept of the mole
- use the mole concept to calculate:
  - number of particles
  - moles of a substance
  - molar mass
  - mass of a substance
- explain the relationship between the mass, moles and molar mass of a substance.

FIGURE 9.2.1 Each of these ice cubes contains more than 10^{23} water (H_2O) molecules. Molecules and atoms are so small that it would be very inconvenient to always count them individually.

It is often essential for chemists to be able to measure an exact number of particles of an element or compound. However, the particles in elements and compounds are so small that it would be difficult to count atoms, ions or molecules individually or even by the thousands of millions. If it were possible to count individual particles, the numbers in even very small samples would be huge and very inconvenient to work with.

The ice cubes shown in Figure 9.2.1 each contain more than 10^{23} water molecules (H_2O). As each water molecule is composed of two hydrogen atoms and one oxygen atom, the number of individual atoms in each ice cube is even higher. A quantity that allows chemists to measure accurate amounts of extremely small particles is required. In this module, you will learn about the very convenient quantity used by chemists—the mole.

WHAT IS A MOLE?

FIGURE 9.2.2 Twelve eggs is one dozen, 24 eggs is two dozen and six eggs is half a dozen.

A dozen is a convenient quantity for buying the eggs shown in Figure 9.2.2. For atoms, ions and molecules, a quantity that describes a much larger number is needed. The accepted quantity for chemists is the **mole.**

One mole contains exactly $6.02214076 \times 10^{23}$ elementary entities, such as atoms, molecules, ions, electrons or other specified particles or items. That is 602 214 076 000 000 000 000 000 items! This number is commonly rounded to 6.02×10^{23} and is referred to as **Avogadro's number.** You may have noticed that Avogadro's number is written in scientific notation. You can revise your understanding of scientific notation in Chapter 1 of your eBook.

Chemists use the mole as a counting unit. It is the standard SI unit for quantifying the amount of matter. Figure 9.2.3 shows some other, non-SI, counting units that you may be familiar with, such as a pair, a dozen or a ream. Table 9.2.1 shows how the use of a mole is similar to that of a dozen, allowing chemists to quantify extremely large numbers of particles in a manageable way, similar to how a dozen quantifies 12 items.

FIGURE 9.2.3 Convenient counting units that you may be familiar with. A pair of shoes equals two, a dozen roses equals 12, a ream of paper equals 500 sheets.

TABLE 9.2.1 Similarity between the use of the dozen and the mole as counting units

Dozen	Mole
1 dozen = 12	1 mole = 6.02×10^{23}
½ dozen = $0.5 \times 12 = 6$	½ mole = $0.5 \times 6.02 \times 10^{23} = 3.01 \times 10^{23}$
0.25 dozen = $0.25 \times 12 = 3$	0.25 moles = $0.25 \times 6.02 \times 10^{23} = 1.51 \times 10^{23}$
2 dozen = $2 \times 12 = 24$	2 moles = $2 \times 6.02 \times 10^{23} = 1.204 \times 10^{24}$
20 dozen = $20 \times 12 = 240$	20 moles = $20 \times 6.02 \times 10^{23} = 1.204 \times 10^{25}$

Later in this module you will learn how to use the mole to calculate the number of particles present in a substance. In calculations, the number of moles is given the symbol n. The unit mole is written in short form as **mol** (similar to the way that the kilogram is written as kg).

AVOGADRO'S CONSTANT

As described above, 1 mole contains exactly $6.02214076 \times 10^{23}$ elementary entities. This number is Avogadro's number. It is based on **Avogadro's constant**, which is $6.02214076 \times 10^{23}$ mol^{-1}. Avogadro's constant has the unit mol^{-1}, whereas Avogadro's number has no unit. Avogadro's constant has the symbol N_A in calculations and is often rounded to 3 significant figures: 6.02×10^{23} mol^{-1}. It is named in honour of Italian scientist Amedeo Avogadro (1776–1856) who developed a hypothesis, now known as Avogadro's law, that states that equal volumes of gases at a given temperature and pressure contain the same number of molecules.

It is very difficult to imagine just how big Avogadro's number really is. Here are some examples to help.

- 6.02×10^{23} grains of sand, placed side by side, would stretch from Earth to the Sun and back about 7 million times.
- A computer counting 10 billion times every second would take nearly 2 million years to reach 6.02×10^{23}.
- 6.02×10^{23} of the marshmallows shown in Figure 9.2.4 would cover Australia to a depth of 900 km!

Avogadro's number is an enormous number, but 1 mole of most elements and compounds will have a small mass and volume. This is due to the extremely small size and mass of atoms, ions and molecules. For example, 1 mole of water has a volume of approximately 18 mL and a mass of approximately 18 g (Figure 9.2.5). The pile of table salt (sodium chloride) in Figure 9.2.5 also represents 1 mole and has a mass of approximately 58 g. It has a different mass to the water sample but has the same number of entities. For water, one entity is one molecule. For the ionic compound sodium chloride, one entity is one formula unit (one sodium ion and one chlorine ion).

INFORMATION PROVIDED BY FORMULAS

When referring to a mole of a substance, it is important to indicate which particle is being specified. In Chapter 8, you learnt that an oxygen molecule contains two oxygen atoms joined by covalent bonding. Figure 9.2.6 shows four different ways that chemists represent the oxygen molecule.

The expression, 'one mole of oxygen' is ambiguous because it could describe 1 mole of oxygen atoms (O) or 1 mole of oxygen molecules (O_2). As there are two atoms in each oxygen molecule, 1 mole of oxygen molecules will contain 2 moles of oxygen atoms. The **molecular formula** of a substance indicates the number of atoms of each element in one molecule of a substance. Some other examples of the use of the mole as a counting unit are provided in Table 9.2.2 on page 180.

The mole is the SI unit of amount of substance. One mole contains exactly $6.02214076 \times 10^{23}$ elementary entities. This number is called Avogadro's number, and it is the fixed numerical value of Avogadro's constant, N_A, when the constant is expressed in mol^{-1}.

FIGURE 9.2.4 One mole of any substance contains 6.02×10^{23} elementary entities (atoms, molecules, ions, electrons or other specified particles or items).

FIGURE 9.2.5 One mole of sodium chloride and one mole of water contain the same number of entities, 6.02×10^{23}.

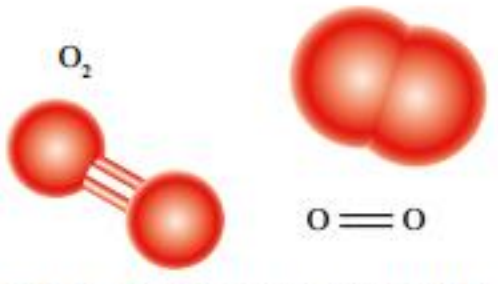


FIGURE 9.2.6 Four different ways chemists represent the oxygen molecule: a formula (O_2), a structural formula (O=O) and two coloured molecular models. Each formula or model shows that one oxygen molecule contains two oxygen atoms.

TABLE 9.2.2 Examples of the use of the mole as a counting unit

Number of moles of element or compound	Information that can be obtained about numbers of particles
1 mole of hydrogen atoms (H)	1 mole of hydrogen atoms (H)
1 mole of hydrogen molecules (H_2)	1 mole of hydrogen molecules (H_2) 2 moles of hydrogen atoms (H)
2 moles of aluminium atoms (Al)	2 moles of aluminium atoms (Al)
2 moles of calcium fluoride (CaF_2)	2 moles of Ca^{2+} ions 4 moles of F^- ions
10 moles of glucose ($C_6H_{12}O_6$) molecules	10 moles of glucose ($C_6H_{12}O_6$) molecules 60 moles of carbon atoms 120 moles of hydrogen atoms 60 moles of oxygen atoms

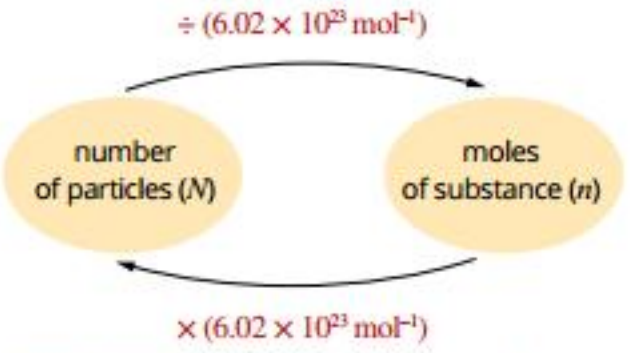


FIGURE 9.2.7 Relationship between number of particles and amount of substance in moles.

CALCULATIONS USING THE MOLE CONCEPT

So far this module has described several different things:

- the mole, which is the SI unit for the amount of substance, abbreviated as **mol**
- the number of moles of substance in a sample, represented in calculations by the symbol n
- Avogadro's constant, $N_A = 6.02 \times 10^{23}\,mol^{-1}$, which is the number of particles per mole
- the actual number of particles in a sample, represented in calculations by the symbol N.

As shown in Figure 9.2.7, there is a mathematical relationship that exists between these quantities. This relationship can be written as the formula:

$$N = n \times N_A$$

Rearranging to make the number of moles the subject:

$$n = \frac{N}{N_A}$$

Considering units, these equations can be represented slightly differently as:

$$N = n\,mol \times 6.02 \times 10^{23}\,mol^{-1}$$

and

$$n\,mol = \frac{N}{6.02 \times 10^{23}\,mol^{-1}}$$

The mole–particle relationship can be used to perform chemical calculations. If the number of moles of a substance is known, then it allows the number of particles to be calculated. Conversely, if the number of particles is known, then the number of moles can be calculated.

Worked example 9.2.1

CALCULATING THE NUMBER OF MOLECULES

Calculate the number of molecules in 3.5 mol of water (H_2O).	
Thinking	**Working**
List the data given in the question next to the appropriate symbol. Include units.	The number of water molecules is the unknown, so: $N(H_2O) = ?$ $n(H_2O) = 3.5\,mol$ $N_A = 6.02 \times 10^{23}\,mol^{-1}$

Rearrange the formula to make the unknown the subject.	$n = \frac{N}{N_A}$ so $N(H_2O) = n(H_2O) \times N_A$
Substitute in the data and solve for the answer.	$N(H_2O) = n(H_2O) \times N_A$ $= 3.5 \times 6.02 \times 10^{23}$ $= 2.1 \times 10^{24}$ Therefore, there are 2.1×10^{24} molecules of H_2O in 3.5 moles of H_2O.

A mole is a convenient unit for counting particles. The number of moles is given the symbol *n* in calculations and the unit is written as mol.

➤ Try yourself 9.2.1

CALCULATING THE NUMBER OF MOLECULES

Calculate the number of molecules in 1.6 mol of carbon dioxide (CO_2).

Worked example 9.2.2

CALCULATING THE NUMBER OF ATOMS

Calculate the number of oxygen atoms in 2.5 mol of oxygen gas (O_2).

Thinking	Working
List the data given in the question next to the appropriate symbol. Include units.	The number of oxygen atoms is the unknown, so: $N(O) = ?$ $n(O_2) = 2.5\,\text{mol}$ $N_A = 6.02 \times 10^{23}\,\text{mol}^{-1}$
Calculate the number of moles of oxygen atoms from the number of moles of oxygen molecules and the molecular formula.	$n(O) = n(O_2) \times 2$ $= 2.5 \times 2$ $= 5.0\,\text{mol}$
Rearrange the formula to make the unknown the subject.	$n = \frac{N}{N_A}$ so $N(O) = n(O) \times N_A$
Substitute in the data and solve for the answer.	$N(O) = n(O) \times N_A$ $= 5.0 \times 6.02 \times 10^{23}$ $= 3.0 \times 10^{24}$ Therefore, there are 3.0×10^{24} O atoms in 2.5 moles of O_2.

➤ Try yourself 9.2.2

CALCULATING THE NUMBER OF ATOMS

Calculate the number of hydrogen atoms in 0.35 mol of methane (CH_4).

Worked example 9.2.3

CALCULATING THE NUMBER OF MOLES OF PARTICLES GIVEN THE NUMBER OF PARTICLES

Calculate the number of moles of ammonia molecules (NH_3) represented by 2.5×10^{22} ammonia molecules.	
Thinking	**Working**
List the data given in the question next to the appropriate symbol. Include units.	The number of moles of ammonia molecules is the unknown, so: $n(NH_3) = ?\,mol$ $N(NH_3) = 2.5 \times 10^{22}$ molecules $N_A = 6.02 \times 10^{23}\,mol^{-1}$
Rearrange the formula to make the unknown the subject.	$n = \frac{N}{N_A}$ n is the unknown so rearrangement is not required
Substitute in the data and solve for the answer.	$n(NH_3) = \frac{N(NH_3)}{N_A}$ $= \frac{2.5 \times 10^{22}}{6.02 \times 10^{23}}$ $= 0.042\,mol$ Therefore, 2.5×10^{22} NH_3 molecules represents 0.042 moles of NH_3.

➤ Try yourself 9.2.3

CALCULATING THE NUMBER OF MOLES OF PARTICLES GIVEN THE NUMBER OF PARTICLES

Calculate the number of moles of magnesium atoms represented by 8.1×10^{20} magnesium atoms.

SKILLBUILDER 9.2.1

Significant figures

The accuracy of an answer in chemistry calculations is limited by the accuracy of the information given. An answer will have the same number of significant figures as there are in the least accurate piece of information. In Worked example 9.2.3, the number of molecules was given to 2 significant figures, therefore the number of moles in the final answer should also be expressed to 2 significant figures. (See Chapter 1 in your eBook for a more detailed treatment of significant figures.)

Worked example 9.2.4

CALCULATING THE NUMBER OF MOLES OF ATOMS GIVEN THE NUMBER OF MOLES OF MOLECULES

Calculate the number of moles of hydrogen atoms in 3.6 mol of sulfuric acid (H_2SO_4).	
Thinking	**Working**
List the data given in the question next to the appropriate symbol. Include units.	The number of moles of hydrogen atoms is the unknown, so: $n(H) = ?\,mol$ $n(H_2SO_4) = 3.6\,mol$
Calculate the number of moles of hydrogen atoms from the amount of sulfuric acid molecules and the molecular formula.	$n(H) = n(H_2SO_4) \times 2$ $= 3.6 \times 2$ $= 7.2\,mol$

➤ Try yourself 9.2.4

CALCULATING THE NUMBER OF MOLES OF ATOMS GIVEN THE NUMBER OF MOLES OF MOLECULES

Calculate the number of moles of hydrogen atoms in 0.75 mol of water (H_2O).

MOLAR MASS

Chemists have cleverly defined the mole so that the mass of 1 mole of an element is closely related to its relative atomic mass. The relative atomic mass of carbon is 12.01, and 1 mole of carbon (6.02×10^{23} atoms) has a mass of 12.01 g. Chemical laboratories always contain a balance like the one in Figure 9.2.8, which is used for weighing samples. If a sample is weighed, the amount in moles can be calculated.

FIGURE 9.2.8 A digital balance is a simple piece of laboratory equipment used for weighing samples.

The mass, in grams, of 1 mole of a particular element or compound is known as its **molar mass**. It is given the symbol M and the unit $g\,mol^{-1}$.

The particles of different elements and compounds have different masses. Therefore, the masses of 1 mole of different elements or compounds will also be different. This is like saying that the mass of one dozen oranges will be greater than the mass of one dozen mandarins because one orange is heavier than one mandarin.

Table 9.2.3 shows that the relative atomic mass of magnesium is approximately double that of carbon, while the relative atomic mass of titanium is almost four times that of carbon. This ratio is retained in the molar masses, where 1 mole of magnesium will be approximately twice the mass of 1 mole of carbon, and 1 mole of titanium will be almost four times the mass of 1 mole of carbon. The relative atomic (or molecular or formula) mass and molar mass have the same magnitude, but molar mass is the only one of these quantities to have a unit, $g\,mol^{-1}$.

TABLE 9.2.3 Relationship between relative atomic mass and molar mass

Element	Relative atomic mass	Molar mass
carbon	12.01	$12.01\,g\,mol^{-1}$
magnesium	24.3	$24.3\,g\,mol^{-1}$
titanium	47.87	$47.87\,g\,mol^{-1}$

Table 9.2.4 shows you how to calculate the molar masses of some common substances. From this table, you can see that 1 mole of each substance has a different mass. Figure 9.2.9 on page 184 is a photograph of 1 mole of some common substances.

TABLE 9.2.4 Calculating the molar mass of a substance by adding the relative atomic masses for each atom present in the substance, based on the molecular or ionic formula

Substance	Relative atomic masses	Molar mass of substance
Na	Na: 22.99	$= 22.99\,g\,mol^{-1}$
O_2	O: 16.00	$= 2 \times 16.00$ $= 32.00\,g\,mol^{-1}$
H_2O	H: 1.01 O: 16.00	$= (2 \times 1.01) + 16.00$ $= 18.02\,g\,mol^{-1}$
CO_2	C: 12.01 O: 16.00	$= 12.01 + (2 \times 16.00)$ $= 44.01\,g\,mol^{-1}$
$NaNO_3$	Na: 22.99 N: 14.01 O: 16.00	$= 22.99 + 14.01 + (3 \times 16.00)$ $= 85.00\,g\,mol^{-1}$

The molar mass of an element is equivalent to the mass of 1 mole of the element. The molar mass of a compound is equivalent to the mass of 1 mole of the compound. It is equal to the relative molecular mass or relative formula mass of the compound expressed in grams per mole. The molar mass is given the symbol, M, and the unit, $g\,mol^{-1}$.

FIGURE 9.2.9 One mole of each substance has a different mass.

MOLE-MASS CALCULATIONS

It is possible to calculate the number of moles in a sample if the mass and molar mass are known. Figure 9.2.10 shows that there is a relationship between mass and number of moles.

carbon: 1 mole is approximately 12 g		
6 g is $\frac{6}{12}$ = 0.5 mol	12 g is $\frac{12}{12}$ = 1 mol	36 g is $\frac{36}{12}$ = 3 mol

FIGURE 9.2.10 The number of moles of a substance is related to the mass of the sample.

This relationship between the number of moles of a substance (n), its molar mass (M) and the mass of the substance (m) can be summarised with the following formula:

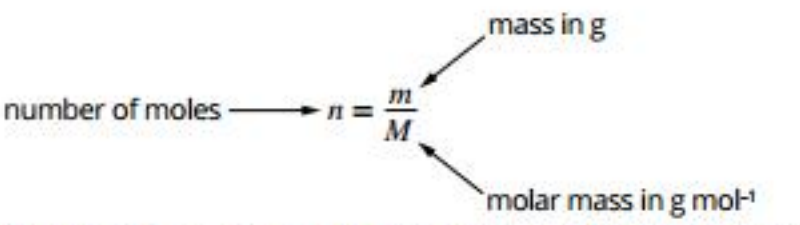


FIGURE 9.2.11 The number of moles in a sample of a substance equals the mass of the sample divided by the molar mass of the substance.

The formula in Figure 9.2.11 can be rearranged to calculate the mass in a sample:

$$m = n \times M$$

The mass of a sample (m) in grams is equal to the number of moles (n) in the sample multiplied by its molar mass (M) in grams per mole.

Worked example 9.2.5

CALCULATING THE MASS OF A SUBSTANCE

Calculate the mass of 0.35 mol of magnesium nitrate ($Mg(NO_3)_2$) to 2 significant figures.	
Thinking	**Working**
List the data given in the question next to the appropriate symbol. Include units. Remember that whenever you are given a formula, you can calculate the molar mass.	$m(Mg(NO_3)_2) = ?\,g$ $n(Mg(NO_3)_2) = 0.35\,mol$ $M(Mg(NO_3)_2) = 24.30 + (2 \times 14.01) + (6 \times 16.00)$ $= 148.32\,g\,mol^{-1}$
Calculate the mass of magnesium nitrate using: $n = \frac{m}{M}$ by rearranging the formula to get: $m = n \times M$	$m = n \times M$ $m(Mg(NO_3)_2) = 0.35 \times 148.32$ $= 51.9155\,g$ $= 52\,g$ to 2 significant figures

➤ Try yourself 9.2.5

CALCULATING THE MASS OF A SUBSTANCE

Calculate the mass of 4.68 mol of sodium carbonate (Na_2CO_3) to 3 significant figures.

The relationship between the number of moles and molar mass of a substance allows you to determine the number of moles of the substance or quantity of atoms present by weighing the substance. This is because the number of particles present in a substance is equal to the number of moles of the substance multiplied by 6.02×10^{23}. Some calculations require you to use both the formulas: $n = \frac{m}{M}$ and $n = \frac{N}{N_A}$.

Worked example 9.2.6

CALCULATING THE NUMBER OF MOLECULES

Calculate the number of CO_2 molecules present in 22 g of carbon dioxide.	
Thinking	**Working**
List the data given in the question next to the appropriate symbol. Include units. Convert mass to grams if required. Remember that whenever you are given a formula, you can calculate the molar mass.	$N(CO_2) = ?$ $M(CO_2) = 12.01 + (2 \times 16.00)$ $= 44.01\,g\,mol^{-1}$ $m(CO_2) = 22\,g$
Calculate the number of moles of CO_2 using: $n = \frac{m}{M}$	$n(CO_2) = \frac{m}{M}$ $= \frac{22}{44.01}$ $= 0.50\,mol$
Calculate the number of CO_2 molecules using: $n = \frac{N}{N_A}$ by rearranging the formula to get: $N = n \times N_A$	$N = n \times N_A$ $N(CO_2) = 0.50 \times 6.02 \times 10^{23}$ $= 3.0 \times 10^{23}$ Therefore, there are 3.0×10^{23} CO_2 molecules in 22 g of CO_2.

➤ Try yourself 9.2.6

CALCULATING THE NUMBER OF MOLECULES

Calculate the number of sucrose molecules in a teaspoon (4.2 g) of sucrose ($C_{12}H_{22}O_{11}$).

9.2 Review

SUMMARY

- The mole is a convenient unit for counting particles. The number of moles is given the symbol *n* and the unit is written as mol.
- The mole is the SI unit of amount of substance. One mole contains exactly $6.02214076 \times 10^{23}$ elementary entities. This number is called Avogadro's number. It is the fixed numerical value of Avogadro's constant, N_A, when the constant is expressed in mol^{-1}.
- The number of particles in 1 mole is known as Avogadro's number and has the numerical value of 6.02×10^{23}.
- The formula $n = \frac{N}{N_A}$ can be used or rearranged to calculate the amount or number of specified particles in a sample. In this formula, n = number of moles (mol), N = number of particles, and N_A = Avogadro's constant (mol^{-1}), which has a value of $6.02 \times 10^{23}\,mol^{-1}$.
- The molar mass of an element or compound is the mass, in grams, of 1 mole of that element or compound. Molar mass is given the symbol *M* and the unit $g\,mol^{-1}$.
- The molar mass of an element or compound has the same numerical value as the relative mass of the element or compound.
- The formula $n = \frac{m}{M}$ can be used or rearranged to calculate the mass (m), moles (n) or molar mass (M) of an element or compound.

KEY QUESTIONS

Describe

1 **a** What does the symbol N_A stand for?
b What is its accepted value?
c How is N_A different to N?

2 Describe the concept of the mole.

3 Indicate if the following statement is true or false.
Molar mass is given the symbol m and the unit $g\,mol^{-1}$.

4 State the formula used to calculate the moles of a substance from a given mass.

5 Complete the table below.

Symbol	Represents
n	
N	
N_A	
M	
m	

Apply

6 Express these numbers to 3 significant figures.
a 0.07676
b 545300

7 Explain why the expression 'one mole of chlorine' is ambiguous.

8 **a** Why does the mass of 1 mole of hydrogen atoms differ from the mass of 1 mole of helium atoms?
b Approximately, how much heavier is 1 mole of helium atoms than 1 mole of hydrogen atoms?

9 A sample of carbon dioxide contains 1 mole of atoms. Does this sample contain 1 mole of carbon dioxide? Justify your answer.

10 Describe how n represents a different quantity to N.

11 Describe how the molar mass of a compound is calculated.

Analyse

12 Determine the number of moles of atoms in 5 moles of water.

13 Consider a 5 mole sample of calcium carbonate, $CaCO_3$.
a Show how each of the following questions leads to a different answer.
i Determine the number of moles of calcium ions in the sample.
ii Determine the number of moles of ions in the sample.
iii Determine the number of moles of atoms in the sample.
iv Determine the number of moles of oxygen atoms in the sample.

b Show how the answers to the following two questions differ.
- **i** Determine the number of moles of calcium atoms in the sample.
- **ii** Determine the number of calcium atoms in the sample.

14 Calculate the following quantities using the relationship between moles and the number of particles.
- **a** number of atoms in 2.0 moles of sodium atoms (Na)
- **b** number of molecules in 0.10 moles of nitrogen molecules (N_2)
- **c** number of atoms in 1.0×10^{-2} moles of iron atoms (Fe)
- **d** number of molecules in 4.62×10^{-5} moles of CO_2 molecules

15 Calculate the number of moles represented by the following using the relationship between moles and the number of particles.
- **a** 3.0×10^{23} molecules of water (H_2O)
- **b** 1.5×10^{23} atoms of neon (Ne)
- **c** 4.2×10^{25} atoms of iron (Fe)

16 **a** Using the relationship between the number of moles and the number of particles, calculate the number of moles of:
- **i** sodium atoms represented by 1.0×10^{20} sodium atoms
- **ii** aluminium atoms represented by 1.0×10^{20} aluminium atoms
- **iii** chlorine molecules represented by 1.0×10^{20} chlorine molecules

Remember: Avogadro's constant, N_A, is $6.02 \times 10^{23}\ mol^{-1}$.

b For the three samples in part **a**, will their masses be the same or different? Will their volume be the same or different? Explain your answers.

17 A sample of nitrogen dioxide, NO_2, contains 5.42×10^{24} atoms. Calculate the number of moles of NO_2 in this sample.

18 Calculate the number of moles of the following using the relationship between moles and the number of particles.
- **a** chlorine atoms in 0.4 mol of chlorine (Cl_2)
- **b** hydrogen atoms in 1.2 mol of methane (CH_4)
- **c** hydrogen atoms in 0.12 mol of ethane (C_2H_6)
- **d** oxygen atoms in 1.5 mol of sodium sulfate (Na_2SO_4)

19 Calculate the molar mass of the following substances.
- **a** nitrogen (N_2)
- **b** ammonia (NH_3)
- **c** sulfuric acid (H_2SO_4)
- **d** iron(III) nitrate ($Fe(NO_3)_3$)
- **e** ethanoic acid (CH_3COOH)
- **f** sulfur atoms (S)
- **g** vitamin C (ascorbic acid, $C_6H_8O_6$)
- **h** hydrated copper(II) sulfate ($CuSO_4.5H_2O$)

20 Calculate the following masses using the relationship between mass, moles and molar mass.
- **a** 1.0 mol of sodium atoms (Na)
- **b** 2.0 mol of oxygen molecules (O_2)
- **c** 0.10 mol of methane molecules (CH_4)
- **d** 0.25 mol of aluminium oxide (Al_2O_3)

21 Calculate the number of moles of these substances using the relationship between mass, moles and molar mass.
- **a** H atoms in 5.0 g of hydrogen (H_2)
- **b** H_2 molecules in 5.0 g of hydrogen (H_2)
- **c** Al atoms in 2.7 g of aluminium (Al)
- **d** CH_4 molecules in 0.40 g of methane (CH_4)
- **e** O_2 molecules in 0.10 g of oxygen (O_2)
- **f** O atoms in 0.10 g of oxygen (O_2)
- **g** P_4 molecules in 1.2×10^{-3} g of phosphorus (P_4)
- **h** P atoms in 1.2×10^{-3} g of phosphorus (P_4)

22 Apply the relationship between number of particles and moles with the relationship between mass, moles and molar mass to calculate the number of atoms in the following substances.
- **a** 23 g of sodium (Na)
- **b** 4.0 g of argon (Ar)
- **c** 0.243 g of magnesium (Mg)
- **d** 10.0 g of gold (Au)

23 Apply the relationship between number of particles and moles with the relationship between mass, moles and molar mass to calculate the:
- **a** number of molecules in
  - **i** 16 g of oxygen (O_2)
  - **ii** 2.8 g of nitrogen (N_2)
- **b** number of oxygen atoms in 3.2 g of sulfur dioxide (SO_2)
- **c** total number of atoms in 288 g of ammonia (NH_3)

9.3 Percentage composition and empirical formulas

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the concept of percentage composition
- calculate percentage composition for a compound
- explain why empirical formulas express the simplest whole number ratio of elements in a compound
- explain the difference between the empirical and molecular formulas for a molecular compound
- determine the empirical formula using data on percentage composition
- determine the molecular formula for a molecular compound based on its molar mass and empirical formula.

Compounds are substances that contain two or more different elements combined in the same fixed proportion by mass. Consider the compound carbon dioxide, depicted in Figure 9.3.1. A single molecule of carbon dioxide consists of one carbon atom bonded to two oxygen atoms. Likewise, 1 mole of carbon dioxide is made up of 1 mole of carbon atoms and 2 moles of oxygen atoms. The relative proportions of the atoms that make up the compound are expressed in its formula, CO_2.

The formulas of compounds are an important part of the language of chemistry. Formulas are used to represent substances. They represent the type and proportion of atoms in a substance. They are particularly useful when writing chemical equations.

While formulas represent the proportions of the atoms in a substance, in the laboratory substances are commonly measured by their mass. The formula does not show the proportional mass of the elements in a compound. If you consider the example of CO_2, the ratio of carbon to oxygen atoms by number is 1:2. However, Figure 9.3.1 shows that carbon and oxygen have different atomic masses, so the ratio by mass is approximately 12:32. The mass ratio is used to determine the **percentage composition** of the substance.

1 mole O	1 mole C	1 mole O
16.00 g O	12.01 g C	16.00 g O

FIGURE 9.3.1 This is a molecular model of a single molecule of carbon dioxide (CO_2), with one carbon atom (black) bonded to two oxygen atoms (red).

PERCENTAGE COMPOSITION

The percentage composition of a given compound tells you the proportion by mass of the different elements in that compound. The proportion of each element is expressed as a percentage of the total mass of the compound.

Being able to determine percentages by mass is important in chemistry. For example, the bauxite ore which is mined in Weipa in Queensland is refined into aluminium. Bauxite is mostly composed of the chemical aluminium hydroxide which has the formula $Al(OH)_3$. During the refining process, aluminium hydroxide is reacted to produce aluminium oxide (alumina), which is finally converted to aluminium metal.

A company that is producing aluminium from bauxite ore would want to know how much metal can potentially be extracted from a given quantity of ore. The pie chart in Figure 9.3.2 shows that, by mass, the percentage of aluminium in aluminium hydroxide is approximately 35%. This means 35 g can potentially be extracted from every 100 g of ore.

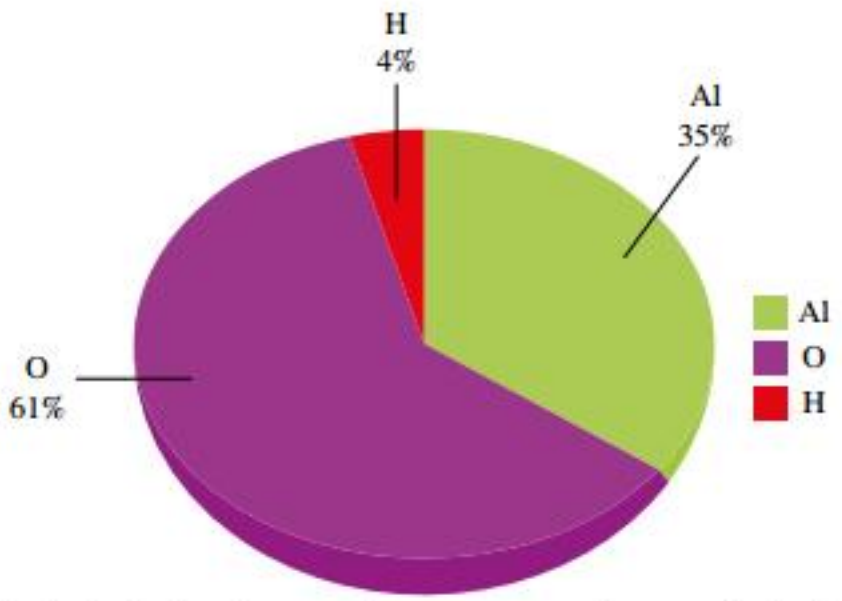


FIGURE 9.3.2 This pie chart shows the percentage composition, by mass, of aluminium hydroxide.

If the chemical formula of a compound is known, the percentage composition can be determined using the molar masses of the elements compared to the molar mass of the compound.

$$\%\text{ by mass of an element in a compound} = \frac{\text{mass of the element in 1 mol of the compound}}{\text{mass of 1 mol of the compound}} \times 100\%$$

Worked example 9.3.1

CALCULATING PERCENTAGE COMPOSITION

Calculate the percentage by mass of aluminium in alumina (Al_2O_3).

Thinking	Working
Find the molar mass of the compound.	$M(Al_2O_3) = (2\times 26.98) + (3\times 16.00)$ $= 101.96\,g\,mol^{-1}$ so 1 mol of the compound has a mass of 101.96 g
Find the total mass of the element in 1 mol of the compound.	mass of Al in 1 mol $= 2\times M(Al)$ $= 2\times 26.98$ $= 53.96\,g$
Find the percentage by mass of the element in the compound.	% by mass of Al in Al_2O_3 $= \frac{\text{mass of Al in 1 mol of } Al_2O_3}{\text{mass of 1 mol of } Al_2O_3} \times 100\%$ $= \frac{53.96}{101.96} \times 100\%$ $= 52.92\%$

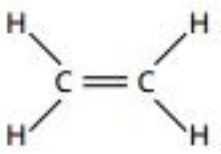
➤ Try yourself 9.3.1

CALCULATING PERCENTAGE COMPOSITION

Calculate the percentage by mass of nitrogen in ammonium nitrate (NH_4NO_3).

EMPIRICAL FORMULAS

Atoms or ions are present in compounds in fixed whole number ratios. The **empirical formula** of a compound gives the simplest whole number ratio of elements in that compound. Table 9.3.1 on page 190 has some examples, including ethene, which has the empirical formula CH_2 and the molecular formula C_2H_4. Ethene is illustrated in Figure 9.3.3.



ethene

FIGURE 9.3.3 Ethene has the empirical formula CH_2 and the molecular formula C_2H_4.

TABLE 9.3.1 Empirical formulas of some common compounds

Compound	Empirical formula	Simplest whole number ratio of elements in the compound
water	H_2O	H : O 2 : 1
ethene (C_2H_4)	CH_2	C : H 1 : 2
calcium carbonate	$CaCO_3$	Ca : C : O 1 : 1 : 3

The empirical formula for a compound is determined from the mass of each element present in a given mass of the compound. These masses can be determined experimentally. Once the masses of elements in a compound are known, the steps in Figure 9.3.4 are followed to convert these masses to a mole ratio—that is, a ratio by number of atoms—and then to an empirical formula.

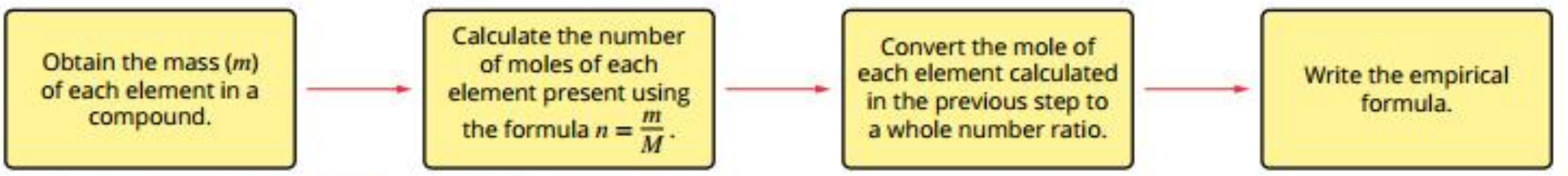

Obtain the mass (m) of each element in a compound.
Calculate the number of moles of each element present using the formula $n = \frac{m}{M}$.
Convert the mole of each element calculated in the previous step to a whole number ratio.
Write the empirical formula.

FIGURE 9.3.4 Steps for calculating an empirical formula.

Worked example 9.3.2

DETERMINING THE EMPIRICAL FORMULA FROM PERCENTAGES

A compound of carbon and oxygen contains 27.3% carbon and 72.7% oxygen by mass. Calculate the empirical formula of the compound.

Thinking	Working
Write down the mass, in grams, of all elements present in the compound. If masses are given as percentages, assume that the sample weighs 100 g, then the percentages become masses in grams.	$m(C) = 27.3\,g$ $m(O) = 72.7\,g$
Calculate the number of moles of each element in the compound using: $n = \frac{m}{M}$	$n(C) = \frac{27.3}{12.01} = 2.28\,mol$ $n(O) = \frac{72.7}{16.00} = 4.54\,mol$
Simplify the ratio by dividing each number of moles by the smallest number of moles calculated in the previous step. This gives you a ratio of the number of atoms of each element.	$\frac{2.28}{2.28} = 1$ $\frac{4.54}{2.28} = 2$
Find the simplest whole number ratio.	1:2
Write the empirical formula.	CO_2

➤ Try yourself 9.3.2

DETERMINING THE EMPIRICAL FORMULA FROM PERCENTAGES

A compound contains 60.3% magnesium and 39.7% oxygen. Calculate the empirical formula of the compound.

Worked example 9.3.3

DETERMINING THE EMPIRICAL FORMULA FROM MASS

A 0.50 g sample of magnesium is heated and allowed to completely react with chlorine. A 1.96 g deposit of white powder is formed. Determine the empirical formula of the compound.

Thinking	Working
Write down the mass, in grams, of all elements present in the compound. If masses are given as percentages, assume that the sample weighs 100 g, then the percentages become masses in grams.	$m(\text{Mg}) = 0.50\,\text{g}$ $m(\text{Cl})$ = total mass of compound sample − mass of Mg $= 1.96 - 0.50$ $= 1.46\,\text{g}$
Calculate the number of moles of each element in the compound using: $n = \frac{m}{M}$	$n(\text{Mg}) = \frac{0.50}{24.31} = 0.0206$ $n(\text{Cl}) = \frac{1.46}{35.5} = 0.0411$
Simplify the ratio by dividing each number of moles by the smallest number of moles calculated in the previous step. This gives you a ratio of the number of atoms of each element.	$\frac{0.0206}{0.0206} = 1$ $\frac{0.0411}{0.0206} = 2$
Find the simplest whole number ratio.	1:2
Write the empirical formula.	$MgCl_2$

➤ Try yourself 9.3.3

DETERMINING THE EMPIRICAL FORMULA FROM MASS

A 16.06 g sample of nitrogen reacts with oxygen to form 62.00 g of a compound containing only nitrogen and oxygen atoms. Determine the empirical formula of the compound.

MOLECULAR FORMULAS

Molecular compounds have a molecular formula in addition to an empirical formula. The molecular formula gives the actual number of atoms of each element present in a molecule, rather than the simplest whole number ratio. The molecular formula can be the same as or different to the empirical formula. The empirical and molecular formulas of some common molecular compounds are shown in Table 9.3.2.

TABLE 9.3.2 Empirical and molecular formulas of some common molecular compounds

Molecule	Molecular formula	Empirical formula
water	H_2O	H_2O
ethane	C_2H_6	CH_3
carbon dioxide	CO_2	CO_2
glucose	$C_6H_{12}O_6$	CH_2O

Ionic compounds do not have molecular formulas because they do not exist as molecules. However, they do have empirical formulas that describe the fixed ratio of ions that exist in their lattices. The formula unit for calcium chloride ($CaCl_2$) is an example of an empirical formula of an ionic compound.

A molecular formula can be determined from the empirical formula of a compound if the molar mass of the compound is also known. The subscripts in a molecular formula of a molecule are always a whole number multiple of the subscripts in the empirical formula. The number of the multiple is determined by the following formula.

$$\text{number of empirical formula units in a molecule} = \frac{\text{molar mass of the compound}}{\text{molar mass of one empirical formula unit}}$$

The general steps to determine a molecular formula are shown in Figure 9.3.5.

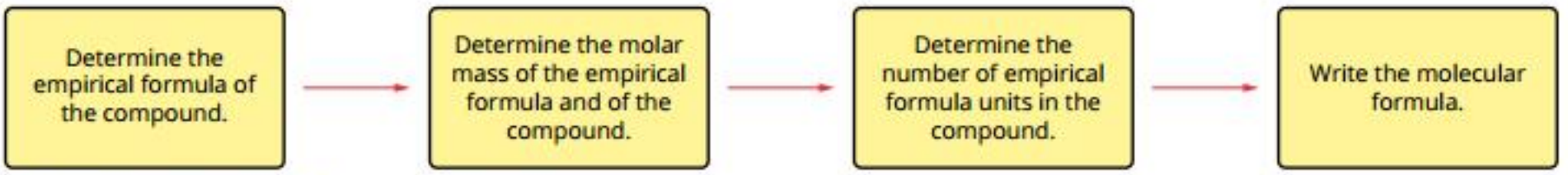

Determine the empirical formula of the compound.
Determine the molar mass of the empirical formula and of the compound.
Determine the number of empirical formula units in the compound.
Write the molecular formula.

FIGURE 9.3.5 Steps for calculating a molecular formula.

Worked example 9.3.4

DETERMINING A MOLECULAR FORMULA

A compound has the empirical formula CH. The molar mass of this compound is $78\,g\,mol^{-1}$. Determine the molecular formula of the compound.

Thinking	Working
Calculate the molar mass of one unit of the empirical formula.	molar mass of a CH unit = 12.01 + 1.01 = $13.03\,g\,mol^{-1}$
Determine the number of empirical formula units in the molecular formula by dividing the molar mass of the compound by the molar mass of the empirical formula unit.	number of CH units = $\frac{78}{13.03}$ = 6
Determine the molecular formula of the compound by multiplying the subscripts of the empirical formula by the number of empirical formula units (calculated in the previous step).	molecular formula = 6 × CH = C_6H_6

➤ Try yourself 9.3.4

DETERMINING A MOLECULAR FORMULA

A compound has the empirical formula C_2H_5. The molar mass of this compound was determined to be $58\,g\,mol^{-1}$. Determine the molecular formula of the compound.

9.3 Review

SUMMARY

- The percentage composition of a given compound tells you the proportion by mass of the different elements in that compound.
- The percentage, by mass, of an element in a compound can be calculated from the mass of the element in 1 mole of the compound and the mass of 1 mole of the compound.
- The empirical formula of a compound gives the simplest whole number ratio of elements in that compound.
- Molecular compounds have a molecular formula that gives the actual number of atoms of each element in the molecule. It may be the same as or different to the empirical formula.
- A molecular formula can be determined from the empirical formula of a compound if the molar mass of the compound is also known.

KEY QUESTIONS

Describe

1 Describe the concept of percentage composition.

2 In which of the following compounds is the molecular formula the same as the empirical formula?
H_2SO_4 H_2O_2 $C_6H_{12}O_6$

Apply

3 Explain why chemical formulas do not directly reflect the percentage composition of a compound.

4 Which two of these compounds have the same empirical formula?
benzene (C_6H_6) ethene (C_2H_4) cyclohexene (C_6H_{10})
ethane (C_2H_6) cyclohexane (C_6H_{12})

5 Nitrogen can form the following three oxides, NO_2, N_2O_4 and N_2O_5. Which of these oxides has the lowest percentage composition of nitrogen?

Analyse

6 Calculate the percentage by mass of the following substances.
- **a** iron in iron(III) oxide (Fe_2O_3)
- **b** uranium in uranium oxide (U_3O_8)
- **c** nitrogen in ammonium chloride (NH_4Cl)
- **d** oxygen in copper(II) nitrate ($Cu(NO_3)_2$)

7 The percentage of oxygen in a dioxide gas is 50%. Which of the following is the gas: CO_2, SO_2 or NO_2?

8 Determine the empirical formulas of the compounds with these percentage compositions.
- **a** 2.74% hydrogen, 97.26% chlorine
- **b** 42.9% carbon, 57.1% oxygen

9 Determine the empirical formulas of the compounds with the following masses.
- **a** 10.0 g of a compound of magnesium and oxygen that contains 6.03 g of magnesium
- **b** 3.2 g of a hydrocarbon that contains 2.4 g of carbon

10 Consider a 100 g sample of ammonia, NH_3.
- **a** Determine the percentage mass of nitrogen in this sample.
- **b** Determine the mass of nitrogen and the mass of hydrogen in this sample.
- **c** What is the mass ratio of nitrogen to hydrogen in this compound?
- **d** What is the ratio of nitrogen atoms to hydrogen atoms by number in NH_3?
- **e** Use your answers to parts **c** and **d** to explain the importance of an understanding of relative masses of elements when manufacturing a chemical such as ammonia.

11 **a** Determine the percentage mass of sodium in table salt, NaCl.
- **b** Determine the mass of sodium and the mass of chlorine required to manufacture 1.00 kg of salt.

12 Determine the molecular formula of the following compounds.

	Empirical formula	Relative molecular mass
a	HO	34
b	CH_2O	90

13 A hydrocarbon contains 85.7% carbon by mass. Its relative molecular mass is 70. Determine the hydrocarbon's:
- **a** empirical formula
- **b** molecular formula

14 A sample of the carbohydrate glucose contains 1.8 g carbon, 0.3 g hydrogen and 2.4 g oxygen.
- **a** Calculate the empirical formula of the compound.
- **b** Deduce its molecular formula given that its relative molecular mass is 180 g mol^{-1}.

9.4 Stoichiometry—chemical equations and the mole

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- write chemical equations using words and formulas
- understand that mass is conserved in chemical reactions and physical transformations
- use coefficients to balance chemical equations
- perform stoichiometric calculations using mole ratios
- determine the mass of an unknown reactant or product using a balanced chemical equation
- calculate limiting and excess reactants
- compare actual yield to theoretical yield.

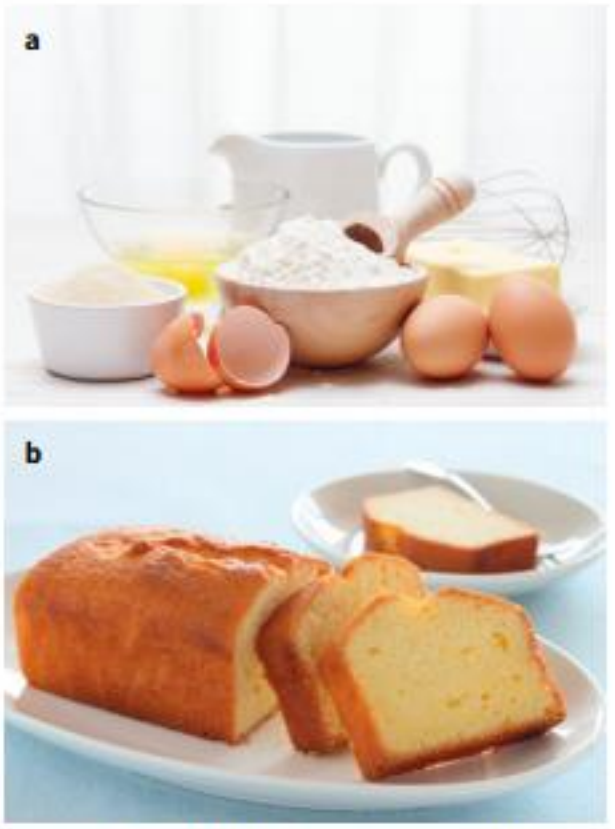


FIGURE 9.4.1 The ingredients needed to bake a simple cake: eggs, sugar, butter, milk and self-raising flour. Chemical reactions occur when a cake is baked.

Chemical reactions are taking place all the time. They occur in the world around you, and even inside your body. In preparing a meal, chemical reactions occur as a result of the cooking process, and after eating the meal your body digests the food and releases its energy through chemical reactions. Plants use chemical reactions to take carbon from the air and turn it into food, and the combustion in a car engine releases the stored energy in fuel.

What do all chemical reactions have in common? The answer is that they involve one or more substances changing into a new substance. Figure 9.4.1 shows the ingredients needed to bake a simple cake: eggs, sugar, butter, milk and self-raising flour. Chemical reactions take place when the ingredients are combined and heated, with the result being a cake! What would you need to do if you wanted to double the mixture? You would need to double every ingredient to maintain the correct proportion. Can you predict from the amounts of ingredients that you have how much cake you will make? Or, if you need to make three cakes, could you determine whether you have enough ingredients in your refrigerator and pantry? That is what this module is about. You will learn how chemical reactions are written, described, balanced and used in calculations.

WRITING CHEMICAL EQUATIONS

A chemical reaction is a change in which one or more **reactants** change into one or more **products**. This change is characterised by the breaking of bonds in the reactants and the formation of bonds in the products. As their names suggest, reactants are the substances present at the start of a reaction, and products are the substances produced in a chemical reaction.

Chemical equations are visual representations that chemists use to describe chemical reactions. To write a chemical equation, you write the names of the reactants on the left and the products on the right, as shown in Figure 9.4.2. An arrow (→) is used to separate the reactants and products, and if you are reading the equation you read the arrow as 'yields'. If there is more than one reactant or product, they are separated with a plus (+) sign.

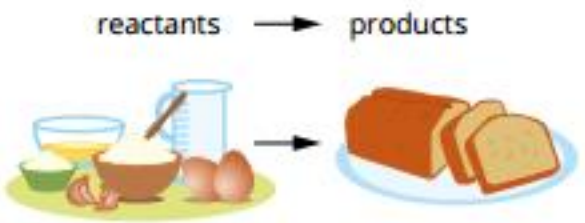


FIGURE 9.4.2 Representing chemical reactions.

Consider the chemical reaction shown in Figure 9.4.3, which shows the **decomposition** of hydrogen peroxide into water and molecular oxygen. In the chemical equation for this reaction, hydrogen peroxide would be on the left because it is the reactant. Water and oxygen would be on the right because they are the products. The equation would be read 'hydrogen peroxide yields water and molecular oxygen'.

Some reactions are complicated, involving many substances that can have long names. For convenience, chemists usually write chemical equations using formulas. The equation (not yet balanced) from Figure 9.4.3 when written with formulas would be:

$$H_2O_2 \rightarrow H_2O + O_2$$

Additional information can be added to chemical equations to indicate physical states, the presence of **catalysts** or the need to supply heat. A catalyst is a substance that speeds up a reaction but is not used up in the reaction. The decomposition of hydrogen peroxide can be catalysed with a chemical called manganese oxide (MnO_2). Table 9.4.1 shows some of the commonly used symbols in chemical equations and their meaning.

TABLE 9.4.1 Symbols used in chemical equations

Symbol	Meaning
(s)	substance is in a solid state; placed after the formula
(l)	substance is in a liquid state; placed after the formula
(g)	substance is in a gaseous state; placed after the formula
(aq)	substance is dissolved in water; placed after the formula
$\rightarrow$	yields
+	used to separate two reactants or two products
$\rightleftharpoons$	used in place of $\rightarrow$ for reversible reactions
$\xrightarrow{\text{heat}}$ or $\xrightarrow{\Delta}$	heat is supplied to the reaction
$\xrightarrow{MnO_2}$	catalyst used; formula of catalyst written above the yield sign

FIGURE 9.4.3 Hydrogen peroxide decomposes to form water and molecular oxygen. In the picture, manganese oxide has been added as a catalyst to speed up the reaction.

Chemical reactions occur when one or more reactants change into one or more products. Chemical equations are used to represent chemical reactions. In a chemical equation, the reactants are written on the left and the products on the right.

If you were to write the equation for the breakdown of hydrogen peroxide with all the additional symbols, it would be:

$$H_2O_2(aq) \xrightarrow{MnO_2} H_2O(l) + O_2(g)$$

BALANCING CHEMICAL EQUATIONS

In a chemical reaction, the total number of each type of atom does not change. If there are a total of two hydrogen atoms that go into a reaction, two hydrogen atoms must come out of the reaction as products. This is because chemical reactions obey the **law of conservation of mass**. The law of conservation of mass states that in any physical change or in any chemical reaction, matter can neither be created nor destroyed.

The total mass of all products is equal to the total mass of all reactants in a chemical reaction.

For a chemical equation to be correct, the number of each type of atom on the reactant side must equal the number of each type of atom on the product side. Therefore, it is a **balanced equation**. Let's again consider the decomposition of hydrogen peroxide:

$$H_2O_2(aq) \xrightarrow{MnO_2} H_2O(l) + O_2(g)$$

If you tally the atoms, there are two hydrogen atoms on each side of the arrow, but there are two oxygen atoms on the reactant side and three oxygen atoms on the product side of the equation. The equation is not balanced. Two molecules of hydrogen peroxide are required for the reaction to produce two water molecules and one oxygen molecule, and this needs to be reflected in the equation.

To write a balanced equation, use coefficients so that the number of each atom on the reactant side equals the number of each atom on the product side.

To write a balanced equation that reflects the correct proportions of reactant and product particles, **coefficients** must be added. Coefficients are whole numbers placed in front of formulas to make the equation balance. Figure 9.4.4 on page 196 shows the balanced equation for the breakdown of hydrogen peroxide.

Unbalanced equation

$$H_2O_2(aq) \xrightarrow{MnO_2} H_2O(l) + O_2(g)$$

Balanced equation

$$2H_2O_2(aq) \xrightarrow{MnO_2} 2H_2O(l) + O_2(g)$$

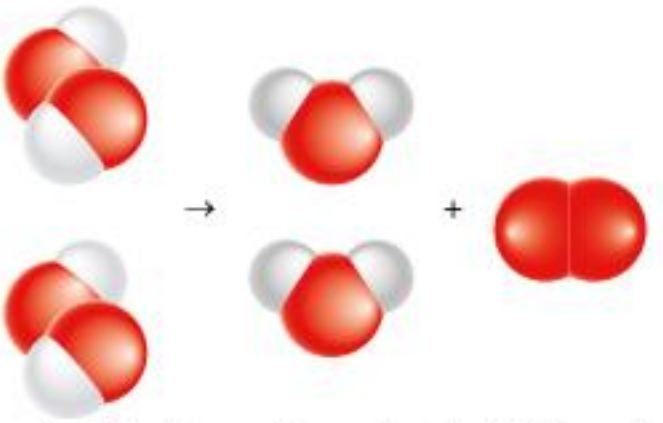


FIGURE 9.4.4 For the equation to be balanced, two molecules of H_2O_2 must react to form two molecules of H_2O and one molecule of O_2. The balanced equation shows the reactant and product molecules in the correct proportion.

SKILLBUILDER 9.4.1

Writing balanced equations

To write a balanced equation, follow these steps.

1 Write an equation in words for the reaction.

aluminium + oxygen gas → aluminium oxide

Reactants are shown to the left of the arrow and products to the right, separated by plus signs where needed.

2 Replace the names of the substances with their correct chemical formulas.

$Al + O_2 \rightarrow Al_2O_3$

Each chemical formula stays the same as you balance the equation. Only the coefficient in front of each formula changes.

3 Balance the elements one at a time using coefficients. You can use common multiples to get the same number of each type of atom on each side of the equation. Trial and error may be necessary to find the best starting point. If the coefficient is 1, then you do not need to write it in the balanced equation.

$Al + O_2 \rightarrow Al_2O_3$

Balancing O: there are 2 oxygen atoms on the left side, and 3 on the right. The lowest common multiple of 2 and 3 is 6, so aim for 6 oxygen atoms on each side. This needs a coefficient of 3 on the left and 2 on the right.

$Al + 3O_2 \rightarrow 2Al_2O_3$

Balancing Al: there is 1 aluminium atom on the left, and 4 on the right. This needs a coefficient of 4 on the left.

$4Al + 3O_2 \rightarrow 2Al_2O_3$

4 Make sure all coefficients are whole numbers. Use the lowest ratio of whole number coefficients.

5 Check the numbers of each type of atom on each side of the equation to make sure that they are equal (i.e. balanced). Add other symbols (such as the state), if known.

$4Al(s) + 3O_2(g) \rightarrow 2Al_2O_3(s)$

Worked example 9.4.1

WRITING A BALANCED EQUATION

Hydrogen and oxygen gas react to form water vapour. The reaction releases energy and is used to fuel rockets. Write a balanced equation for this reaction.	
Thinking	**Working**
Write the equation in words.	hydrogen + oxygen → water
Write correct formulas.	$H_2 + O_2 \rightarrow H_2O$
Balance oxygen.	2 oxygen reactant 1 oxygen product Multiply product H_2O by 2 $H_2 + O_2 \rightarrow 2H_2O$
Balance hydrogen.	2 hydrogen reactant 4 hydrogen product Multiply reactant H_2 by 2 $2H_2 + O_2 \rightarrow 2H_2O$
Check balancing and add state symbols, if known.	2 oxygen reactant 2 oxygen product 4 hydrogen reactant 4 hydrogen product $2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$

➤ Try yourself 9.4.1

WRITING A BALANCED EQUATION

Iron metal and chlorine gas react to form solid iron(III) chloride. Write a balanced equation for this reaction.

Worked example 9.4.2

WRITING A BALANCED EQUATION (MORE DIFFICULT EXAMPLE)

Ethane gas (C_2H_6) readily combusts with oxygen gas to form CO_2 and H_2O. Write a balanced equation for this reaction.	
Thinking	**Working**
Write the equation in words.	ethane + oxygen → carbon dioxide + water
Write correct formulas.	$C_2H_6 + O_2 \rightarrow CO_2 + H_2O$

Balance carbon.	2 carbon reactant 1 carbon product Multiply product CO_2 by 2 $C_2H_6 + O_2 \rightarrow 2CO_2 + H_2O$
Balance hydrogen.	6 hydrogen reactant 2 hydrogen product Multiply product H_2O by 3 $C_2H_6 + O_2 \rightarrow 2CO_2 + 3H_2O$
Balance oxygen. In this example, oxygen is balanced last because one of the substances, O_2, only contains oxygen atoms. To avoid unbalancing the other elements, only change the coefficient of the oxygen molecule.	2 oxygen reactant 7 oxygen product $7 \div 2 = 3.5$, so multiply the O_2 on the left by 3.5 $C_2H_6 + 3.5O_2 \rightarrow 2CO_2 + 3H_2O$
Double to make all coefficients whole numbers.	$2C_2H_6 + 7O_2 \rightarrow 4CO_2 + 6H_2O$
Check balancing and add state symbols, if known.	4 carbon reactant 4 carbon product 12 hydrogen reactant 12 hydrogen product 14 oxygen reactant 14 oxygen product $2C_2H_6(g) + 7O_2(g) \rightarrow 4CO_2(g) + 6H_2O(g)$

➤ **Try yourself 9.4.2**

WRITING A BALANCED EQUATION (MORE DIFFICULT EXAMPLE)

Methanol (CH_4O) readily combusts with oxygen gas to form CO_2 and H_2O. Write a balanced equation for this reaction.

STOICHIOMETRY AND THE MOLE RATIO

Stoichiometric calculations allow you to use the mole ratio established in a chemical equation to predict the amount of a product that will be formed or how much reactant will be used.

The coefficients used to balance chemical equations show the ratios between the reactants and products involved in a reaction. The study of ratios of moles of substances in chemical reactions is called **stoichiometry**. Stoichiometric calculations are based on the law of conservation of mass.

Consider the equation for the precipitation reaction that occurs when a solution of calcium chloride reacts with a solution of silver nitrate:

$$CaCl_2(aq) + 2AgNO_3(aq) \rightarrow 2AgCl(s) + Ca(NO_3)_2(aq)$$

The equation indicates that 1 mole of $CaCl_2$ reacts with 2 moles of $AgNO_3$ to form 2 moles of solid AgCl and 1 mole of $Ca(NO_3)_2$.

In more general terms, the number of moles of $AgNO_3$ that reacts will always be double the number of moles of $CaCl_2$ that reacts. The number of moles of AgCl produced will be equal to the number of moles of $AgNO_3$ used and double the number of moles of $Ca(NO_3)_2$ produced.

You can use the coefficients of this reaction to write relationships that show the **mole ratios** of any two chemicals involved in the reaction:

$$\frac{n(AgNO_3)}{n(CaCl_2)} = \frac{2}{1}, \frac{n(CaCl_2)}{n(AgCl)} = \frac{1}{2} \text{ and } \frac{n(AgCl)}{n(AgNO_3)} = \frac{2}{2} = \frac{1}{1}$$

In the stoichiometric calculations that you will perform in this module, the number of moles or mass of one of the reactants or products will always be known (called the 'known chemical') and is used to determine the number of moles or mass of one of the other reactants or products involved in the reaction (called the 'unknown chemical'). You can write the relationship between the known and the unknown chemicals using ratios:

$$\frac{n(\text{unknown chemical})}{n(\text{known chemical})} = \frac{\text{coefficient of unknown chemical}}{\text{coefficient of known chemical}}$$

> **When carrying out any stoichiometric calculation, you must always clearly state the mole ratio you are working with.**

Worked example 9.4.3

USING MOLE RATIOS

Solutions of copper(II) sulfate and sodium hydroxide are mixed together, forming 0.40 mol of solid copper(II) hydroxide. The products of the reaction are copper(II) hydroxide and sodium sulfate. Calculate how many moles of sodium hydroxide reacted in this reaction.	
Thinking	**Working**
Write a balanced equation for the reaction.	$CuSO_4(aq) + 2NaOH(aq) \rightarrow Cu(OH)_2(s) + Na_2SO_4(aq)$
Determine the number of moles of the 'known chemical' (the one you are provided information about in the question).	$n(Cu(OH)_2) = 0.40$ mol
Find the mole ratio: mole ratio = $\frac{\text{coefficient of unknown chemical}}{\text{coefficient of known chemical}}$ The 'unknown chemical' is the one whose number of moles you need to calculate.	$\frac{\text{coefficient of NaOH}}{\text{coefficient of Cu(OH)}_2} = \frac{2}{1}$
Calculate the number of moles of the unknown chemical using: $n(\text{unknown}) = n(\text{known}) \times (\text{mole ratio})$	$n(NaOH) = 0.40 \times \frac{2}{1}$ $= 0.80$ moles

➤ Try yourself 9.4.3

USING MOLE RATIOS

Solutions of lead(II) nitrate and potassium iodide are mixed together, forming 0.3 mol of solid lead(II) iodide. The products formed are lead(II) iodide precipitate and potassium nitrate solution. Calculate how many moles of potassium iodide reacted in this reaction.

MASS–MASS STOICHIOMETRY

When you carry out a reaction in the laboratory, you will typically measure quantities of chemicals in grams, not moles. For this reason, most calculations will require you to start and finish with mass rather than moles of a substance. As you learnt in Module 9.2, the number of moles of a substance can be calculated from a given mass using the relationship:

$$\text{number of moles} = \frac{\text{mass (in g)}}{\text{molar mass (in g mol}^{-1}\text{)}}$$

This can be written as:

$$n = \frac{m}{M}$$

To calculate a final answer as a mass, this formula is rearranged:

$$m = n \times M$$

There are several steps involved in calculating the mass of an unknown chemical.

1 Write a balanced equation for the reaction.
2 Calculate the number of moles of the known chemical using the formula $n = \frac{m}{M}$.
3 Use the mole ratios in the equation to calculate the number of moles of the second substance.
4 Calculate the mass of the unknown substance using $m = n \times M$.

Figure 9.4.5 provides a flow chart that summarises this process. Worked example 9.4.4 will help you to understand these steps.

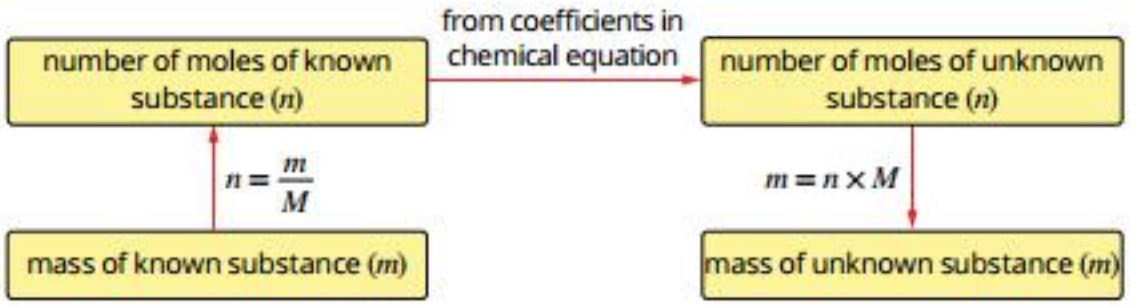

number of moles of known substance (n)
from coefficients in chemical equation
number of moles of unknown substance (n)
$n = \frac{m}{M}$
$m = n \times M$
mass of known substance (m)
mass of unknown substance (m)

FIGURE 9.4.5 A flow chart for mass–mass stoichiometric calculations is helpful when trying to solve these problems.

Worked example 9.4.4

MASS–MASS STOICHIOMETRIC PROBLEMS

Solid magnesium burns in the presence of oxygen gas to form magnesium oxide. Calculate the mass of oxygen that would need to burn to produce 24.0 g of magnesium oxide.

Thinking	Working
Write a balanced equation for the reaction.	$2Mg(s) + O_2(g) \rightarrow 2MgO(s)$
Calculate the number of moles of the known chemical (magnesium oxide): $n = \frac{\text{mass}(m)}{\text{molar mass}(M)}$	$n(MgO) = \frac{24.0\,g}{40.31\,g\,mol^{-1}} = 0.60\,mol$
Calculate the mole ratio: $\text{mole ratio} = \frac{\text{coefficient of unknown chemical}}{\text{coefficient of known chemical}}$	$\frac{\text{coefficient of } O_2}{\text{coefficient of MgO}} = \frac{1}{2}$
Calculate the number of moles of the unknown chemical: $n(\text{unknown}) = n(\text{known}) \times \text{mole ratio}$	$n(O_2) = n(MgO) \times \text{mole ratio} = 0.60 \times \frac{1}{2} = 0.30\,mol$
Calculate the mass of the unknown chemical: $m = n(\text{unknown}) \times \text{molar mass}$	$m(O_2) = 0.30 \times 32.0 = 9.6\,g$

➤ Try yourself 9.4.4

MASS–MASS STOICHIOMETRIC PROBLEMS

A reaction between solutions of sodium sulfate and barium nitrate produces a precipitate of barium sulfate with a mass of 2.440 g. Calculate the mass of sodium sulfate required to produce this precipitate.

LIMITING AND EXCESS REACTANTS

When two reactants are mixed in a chemical reaction, it is unlikely that the reactants are present in the exact mole ratio indicated by the balanced chemical equation. In this case, one of the reactants will be used up before the other and some of the other reactant will be left over at the end of the reaction.

To illustrate this situation simply, first work on a problem that does not involve chemicals. Suppose that you have been given some skateboard decks and wheels and you want to make as many complete skateboards as you can. As you can see in Figure 9.4.6, a complete skateboard is made up of one deck and four wheels.

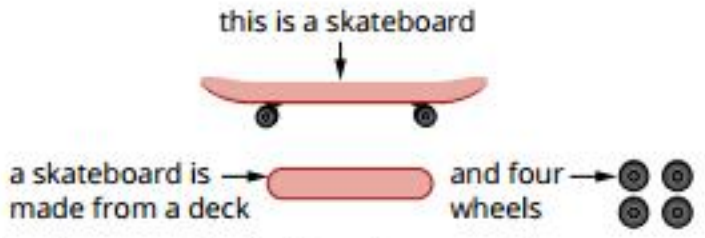


FIGURE 9.4.6 In order to make a complete skateboard, you must always use one deck and four wheels. This sets up the basic formula for a skateboard.

Now consider the situation shown in Figure 9.4.7. If you were given two decks and ten wheels, how many complete skateboards could you make from these materials?

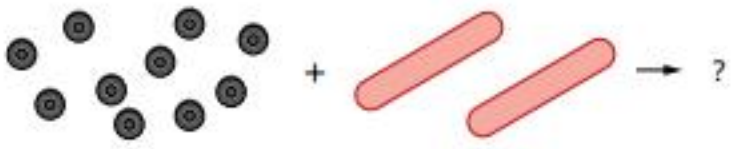


FIGURE 9.4.7 How many complete skateboards can be made with ten wheels and two decks?

The answer is that you could make two complete skateboards and there would be two wheels left over (Figure 9.4.8).

FIGURE 9.4.8 When supplied with two decks and ten wheels, the maximum number of skateboards that can be made is two. There will be two wheels that are not used.

In this example, you can say that the two wheels left at the end were in excess. The total number of complete skateboards you could make was limited by the number of decks available.

A similar situation arises in chemical reactions if the quantities of reactants supplied are not in the exact mole ratio as that shown in the balanced equation for the reaction.

When this happens, the reactant that is:

- completely consumed is the **limiting reactant**
- not completely consumed is the **excess reactant**.

Figure 9.4.9 on page 202 shows three different scenarios for the reaction in which hydrogen gas and oxygen gas combine to form water, according to the equation:

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$$

Each of the diagrams provides examples to illustrate the concepts of limiting and excess reactants.

i In a chemical reaction, the limiting reactant is completely used up.

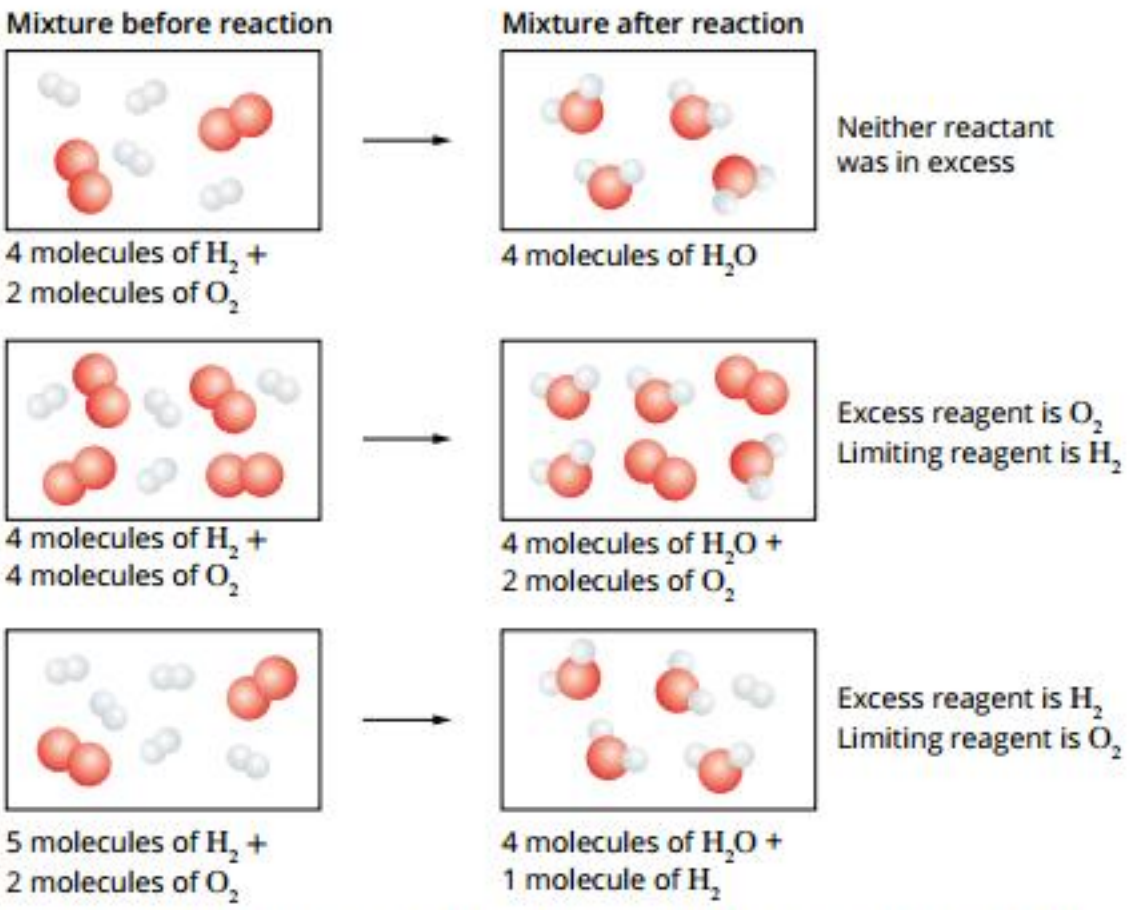

Mixture before reaction
Mixture after reaction
Neither reactant was in excess
4 molecules of H_2 + 2 molecules of O_2
4 molecules of H_2O
Excess reagent is O_2
Limiting reagent is H_2
4 molecules of H_2 + 4 molecules of O_2
4 molecules of H_2O + 2 molecules of O_2
Excess reagent is H_2
Limiting reagent is O_2
5 molecules of H_2 + 2 molecules of O_2
4 molecules of H_2O + 1 molecule of H_2

FIGURE 9.4.9 Different scenarios showing the concept of a limiting reactant for the reaction $2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$

- Note that in each of the examples shown in Figure 9.4.9, the amount of product:
- formed in these types of reactions is determined by the amount of the limiting reactant present in the reaction mixture
- cannot be determined from the amount of excess reactant.

In the skateboard example, it was the number of decks, not the number of wheels, that determined how many complete skateboards could be made. You must always use the amount of the limiting reactant to determine the amount of product that will be formed.

To solve a limiting reactant problem in which you are required to work out the amount of product, there are three main steps.

1 Calculate the number of moles of each reactant.
2 Determine which reactant is in excess and, therefore, which is the limiting reactant.
3 Use the amount of limiting reactant to work out the amount of product formed.

Worked example 9.4.5

MASS–MASS STOICHIOMETRY CALCULATION WITH ONE REACTANT IN EXCESS

A solution containing 20.0 g of dissolved sodium hydroxide is added to a solution containing 25.0 g aluminium nitrate. The balanced equation for the reaction is:
$3NaOH(aq) + Al(NO_3)_3(aq) \rightarrow Al(OH)_3(s) + 3NaNO_3(aq)$

a Determine which reactant is the limiting reactant.

Thinking	Working
Calculate the number of moles of each of the reactants in the equation using: $n = \frac{m}{M}$	For NaOH: $n(NaOH) = \frac{20.0}{39.98} = 0.500\,mol$ For $Al(NO_3)_3$: $n(Al(NO_3)_3) = \frac{25.0}{213.01} = 0.117\,mol$

Use the coefficients of the equation to find the limiting reactant.	The equation shows that 3 mol of NaOH reacts with 1 mol of $Al(NO_3)_3$. So to react all of the $Al(NO_3)$ you will require: $\frac{3}{1} \times n(Al(NO_3)_3)$ of NaOH $\frac{3}{1} \times 0.117 = 0.351\,mol$ As there is 0.500 mol available, the NaOH is in excess. So, $Al(NO_3)_3$ is the limiting reactant (it will be completely consumed) and the amount of $Al(NO)_3$ will therefore determine the amount of product produced.

b Determine the mass of precipitate formed.

Thinking	**Working**
The precipitate formed is $Al(OH)_3$. We therefore need to find the mole ratio of $Al(OH)_3$ (the unknown chemical) to the limiting reactant (the known chemical) using their coefficients: mole ratio = $\frac{\text{coefficient of unknown chemical}}{\text{coefficient of known chemical}}$	$\frac{\text{coefficient of } Al(OH)_3}{\text{coefficient of } Al(NO_3)_3} = \frac{1}{1}$
Calculate the number of moles of the unknown chemical using the number of moles of limiting reactant: n(unknown) = n(limiting reactant) × mole ratio	$n(Al(OH)_3) = n(Al(NO_3)_3) \times \frac{1}{1}$ $= 0.117 \times \frac{1}{1}$ $= 0.117\,mol$
Calculate the mass of the unknown chemical: m(unknown) = n(unknown) × molar mass	molar mass of $Al(OH)_3 = 78.01\,g\,mol^{-1}$ $m(Al(OH)_3) = 0.117 \times 78.01$ $= 9.13\,g$

➤ Try yourself 9.4.5

MASS–MASS STOICHIOMETRY CALCULATION WITH ONE REACTANT IN EXCESS

A solution containing 0.600 g of lead(II) nitrate is added to a solution containing 2.60 g of potassium iodide. The balanced equation for the reaction is:

$$2KI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + 2KNO_3(aq)$$

a Determine which reactant is the limiting reactant.

b Determine the mass of precipitate formed.

YIELD

A major consideration in industrial chemistry is the amount of product that can be produced from given amounts of reactants in a given time. Many industrial processes involve a number of steps to make the final product. At each step, the conversion from reactants to products is usually less than complete. For every step in a reaction pathway, the amount of final product diminishes. Industrial chemists must consider the efficiency of a reaction pathway and the wastes that are produced (Figure 9.4.10 on page 204).

FIGURE 9.4.10 Most chemical reactions carried out in industrial processes are not 100% efficient and so waste chemicals are produced. The reduction or elimination of waste chemicals is a major concern for industrial chemists.

Theoretical yield is the maximum amount of product that can be formed using stoichiometric ratios of the limiting reactant and assumes 100% conversion.

The mass of product that can be formed if all reactants react to produce products according to the reaction equation is known as the **theoretical yield**. The theoretical yield is calculated using the mole ratios of the equation and assumes 100% conversion of the reactants.

In practice, when reactants are mixed together in the correct mole ratio, the amount of product that is actually produced (the **actual yield**) will typically be less than the amounts predicted from stoichiometric calculations. A number of factors can influence the amount of product that will be produced in a given reaction.

- Some reactions do not go to completion. They reach a state of equilibrium, which will be covered in detail in Unit 3. When a reaction reaches equilibrium rather than continuing on to completion, the actual yield will be less than the theoretical yield.
- If the reaction rate is slow, the reaction may not proceed to completion in the time available. This will reduce the actual yield so that the theoretical yield is not obtained.
- Loss of reactants and products during transfers between reaction vessels and in separation and purification stages such as filtration will result in smaller amounts of the product being obtained than expected.
- There may be more than one reaction occurring, meaning that some of the reactants end up forming other products.

Percentage yield

The **percentage yield** compares the actual yield to the theoretical yield. It is a measure of the efficiency of a production process for the particular conditions and method used for the synthesis. The higher the value of the percentage yield, the greater the degree of conversion from reactants to products for the reaction.

Percentage yield can be calculated using the formula:

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times \frac{100}{1}\,\%$$

Worked example 9.4.6

CALCULATING THE PERCENTAGE YIELD OF A REACTION

Aspirin ($C_9H_8O_4$) is made when ethanoic anhydride ($C_4H_6O_3$) reacts with 2-hydroxybenzoic acid ($C_7H_6O_3$). A 12.50 g sample of $C_4H_6O_3$ is reacted with excess 2-hydroxybenzoic acid in the lab to produce 37.80 g of aspirin. The unbalanced equation for the reaction is $C_7H_6O_3 + C_4H_6O_3 \rightarrow C_9H_8O_4 + H_2O$. Calculate the percentage yield of this reaction.

Thinking	Working
Write a balanced equation for the reaction.	$2C_7H_6O_3 + C_4H_6O_3 \rightarrow 2C_9H_8O_4 + H_2O$
Use the formula $n = \frac{m}{M}$ to determine the amount of reactant.	$n(C_4H_6O_3) = \frac{12.50}{102.10}$ $= 0.1224\,\text{mol}$
Use the mole ratio for the reaction to determine the number of moles of the product that would be made if all of the reactant reacted.	$\text{mole ratio} = \frac{\text{coefficient of } C_9H_8O_4}{\text{coefficient of } C_4H_6O_3} = \frac{2}{1}$ $n(C_9H_8O_4) = \frac{2}{1} \times n(C_4H_6O_3)$ $= \frac{2}{1} \times 0.1224$ $= 0.2448\,\text{mol}$
Use the formula $m = n \times M$ to determine the mass of the product if all of the reactant reacts. This is the theoretical yield of the product.	$m(C_9H_8O_4) = n \times M$ $= 0.2448 \times 180.17$ $= 44.11\,\text{g}$
Calculate the percentage yield for this reaction from the formula: $\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times \frac{100}{1}\%$	$\text{percentage yield} = \frac{37.80}{44.11} \times \frac{100}{1}\%$ $= 85.69\%$

➤ Try yourself 9.4.6

CALCULATING THE PERCENTAGE YIELD OF A REACTION

An 80.0 g sample of potassium is reacted with excess chlorine gas to produce 120.2 g of potassium chloride. Calculate the percentage yield of this reaction.

9.4 Review

SUMMARY

- A chemical equation is a representation of a chemical reaction using symbols of the elements to indicate the relative amounts, usually in moles, of each reactant and product.
- The total mass of reactants consumed in a chemical reaction equals the total mass of products formed. This is a consequence of the law of conservation of mass.
- To write a balanced chemical equation, use coefficients so that the number and type of each atom on the reactant side equals the number and type of each atom on the product side.
- A balanced equation shows the ratio of the number of moles of reactants used and products formed in the reaction.
- Given the quantity of one of the reactants or products of a chemical reaction, the quantity of all other reactants and products can be predicted by working through the following steps.
  1 Write a balanced equation for the reaction.
  2 Calculate the number of moles of the known chemical.
  3 Use the mole ratios of reactants and products in the balanced equation to calculate the number of moles of the unknown chemical.
  4 Use the appropriate formula to determine the required quantities of the unknown chemical. The formula is:

$$m = n \times M$$

- The limiting reactant is the reactant that is consumed completely in a chemical reaction.
- The limiting reactant is used to predict the amount of products formed and the amount of excess reactants.
- The theoretical yield of a chemical reaction is the mass of the product that would be formed if the limiting reactant reacted completely as predicted by stoichiometric calculations.
- To calculate the percentage yield, divide the actual yield obtained by the theoretical yield that would be obtained if all of the limiting reactant reacted completely, and multiply by 100%:

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times \frac{100}{1}\%$$

KEY QUESTIONS

Describe

1 Define the term 'chemical equation'.

2 Identify if the following reaction is balanced.

$Zn(OH)_2 + H_3PO_4 \rightarrow Zn_3(PO_4)_2 + H_2O$

3 Define the term 'stoichiometry'.

4 A piece of magnesium is added to hydrochloric acid, HCl, in a plastic bag. The bag is sealed and a reaction producing a gas is evident. What does the law of conservation of mass suggest about the contents of the bag during and after this reaction?

5 Identify if the following statement is true or false.
The reactant that is completely consumed in a chemical reaction is the excess reactant.

6 State the formula for calculating percentage yield.

7 State three reasons why actual yield varies from theoretical yield.

Apply

8 Explain why chemical equations must be balanced.

9 Represent the following reactions with balanced equations.

a Nitrogen and oxygen react in the cylinders of car engines to produce nitrogen monoxide gas.

b Heating tin(IV) hydroxide powder gives solid tin(IV) oxide and water.

c Solid magnesium reacts with aqueous silver nitrate to form solid silver and aqueous magnesium nitrate.

10 Explain how stoichiometric calculations use the mole ratio.

11 The equation for the reaction between hydrogen and oxygen gases is:

$2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$

A reaction uses 1.8 moles of oxygen gas. How many moles of hydrogen gas reacted with the oxygen and how many moles of water formed?

12 The equation for the combustion of ethane is:

$2C_2H_6(g) + 7O_2(g) \rightarrow 4CO_2(g) + 6H_2O(g)$

Calculate the amount of oxygen gas required to react with 0.64 mol of ethane and calculate the amounts of products formed in the reaction.

Analyse

13 The equation for the reaction between aluminium and gaseous hydrochloric acid is:

$2Al(s) + 6HCl(g) \rightarrow 2AlCl_3(s)$

1.2 mol of HCl is reacted with aluminium.

- **a** Calculate the number of moles of aluminium needed to react exactly with the HCl.
- **b** Calculate the number of moles of $AlCl_3$ formed.
- **c** Calculate the mass of $AlCl_3$ formed.

14 8.0 mol of ammonia, NH_3, is formed from a reaction between nitrogen and hydrogen gases. The equation is:

$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$

- **a** Calculate the number of moles of each reactant required for this reaction.
- **b** Calculate the mass of each reactant.

15 A 5.64 g precipitate of calcium phosphate is obtained when a solution of sodium phosphate is added to a solution of calcium nitrate. The balanced equation for the reaction is:

$3Ca(NO_3)_2(aq) + 2Na_3PO_4(aq) \rightarrow Ca_3(PO_4)_2(s) + 6NaNO_3(aq)$

Calculate the mass of calcium nitrate required to produce this precipitate.

16 In three different experiments, different amounts of nitrogen and hydrogen reacted to form ammonia, according to the equation:

$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$

This table shows the amount of the reactants used in each experiment. Determine the amount of each product and the amount of each reactant remaining at the end of the reaction.

Nitrogen molecules available	Hydrogen molecules available	Ammonia molecules produced	Nitrogen molecules in excess	Hydrogen molecules in excess
2	10			
879	477			
9 mol	6 mol			

17 Sodium metal can react with chlorine gas to form sodium chloride. A 25.0 g piece of sodium is reacted with 50.0 g of chlorine gas.

- **a** Write the balanced equation for the reaction between sodium and chlorine.
- **b** Calculate the mass of sodium chloride that will form in the reaction.

18 Sodium hydroxide, NaOH, is a strong base. A waste sample can be neutralised and disposed of safely if dilute. H_2SO_4 solution is added carefully to the NaOH. The equation for the reaction is:

$H_2SO_4(aq) + 2NaOH(s) \rightarrow Na_2SO_4(aq) + 2H_2O(l)$

Calculate the mass of sulfuric acid needed to react with 8.80 g of NaOH.

19 Calculate the percentage yield for the reaction in which 20.0 g of ethanol (C_2H_5OH) is oxidised to produce 21.5 g of ethanoic acid (CH_3COOH) according to the equation:

$$C_2H_5OH \xrightarrow{H^+/Cr_2O_7^{2-}} CH_3COOH$$

(Note: as shown, this equation is not balanced. However, in the balanced equation, the mole ratio between ethanol and ethanoic acid is 1:1.)

20 During a trial experiment for the industrial production of ethanol from ethene, 150 g of ethene was reacted with water to produce ethanol according to the balanced equation:

$C_2H_4(g) + H_2O(g) \rightarrow C_2H_5OH(g)$

Calculate the theoretical yield, in grams, of ethanol for this reaction.

21 The mass of aluminium nitrate in a solution is determined by adding sodium carbonate solution to precipitate the aluminium as aluminium carbonate. The equation for the reaction is:

$2Al(NO_3)_3(aq) + 3Na_2CO_3(aq) \rightarrow Al_2(CO_3)_3(s) + 6NaNO_3(aq)$

In a particular reaction, 4.68 g of precipitate is obtained.

- **a** Calculate the moles of aluminium carbonate produced.
- **b** Determine the required mole ratio for the reaction.
- **c** Calculate the mass of aluminium nitrate that reacted.

22 Potassium iodide and lead(II) nitrate solutions react to form a precipitate of lead(II) iodide:

$2KI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + 2KNO_3(aq)$

In each of the following cases, calculate the quantities required.

- **a** If 1.0 mol of potassium iodide reacts with 1.0 mol of lead(II) nitrate, determine which reactant is in excess and by how many moles.
- **b** If 0.50 mol of potassium iodide reacts with 2.0 mol of lead(II) nitrate, determine which reactant is in excess and by how many moles.
- **c** If 1.00 g of lead(II) nitrate reacts with 1.50 g of potassium iodide, determine which reactant is in excess and the mass of lead(II) iodide that forms.

Chapter review

09

KEY TERMS

actual yield
atomic mass
atomic mass unit (amu)
Avogadro's constant
Avogadro's number
balanced equation
catalyst
chemical equation
chemical reaction
coefficient
decomposition
empirical formula
excess reactant
law of conservation of mass
limiting reactant
mass spectrometry
mole
molar mass
mole
mole ratio
molecular formula
molecule
percentage composition
percentage yield
product
reactant
relative atomic mass
relative formula mass
relative molecular mass
stoichiometry
theoretical yield

KEY QUESTIONS

Describe

1 Select the correct definition for relative atomic mass.
- **A** The mass of 1 mol of the compound. It is equal to the relative molecular or relative formula mass of the compound expressed in grams.
- **B** The mass of one molecule of a substance relative to the mass of a ^{12}C atom taken as exactly 12 amu.
- **C** The weighted average of the atomic masses of isotopes of an element.
- **D** The percentage abundance of an isotope in the natural environment.

2 Define the term 'molar mass'.

3 Define the term 'empirical formula'.

4 A balanced equation requires:
- **A** the mass of solid reactants to equal the mass of solid products
- **B** the same number and type of reactant atoms as product atoms
- **C** the same number of reactant molecules as product molecules
- **D** the total of the reactant coefficients to equal that of the product coefficients

5 Which option will have a relative formula mass?
- **A** He
- **B** N_2
- **C** NO_2
- **D** Li_3N

6 Select the best description of the theoretical yield of a reaction.
- **A** the mass of product formed if the limiting reactant reacts fully
- **B** the mass of product formed in a reasonable amount of time
- **C** the sum of the masses of each reactant
- **D** the total mass of all products formed in the reaction

7 State the law of conservation of mass.

Apply

8 Which one of the following contains 6.02×10^{23} of the particles in bold?
- **A** **hydrogen atoms** in 1 mole of hydrogen gas
- **B** **ions** in 1 mole of NaCl
- **C** **atoms** in 0.2 mol of $CaCO_3$
- **D** **hydrogen atoms** in 0.5 mol of CH_4

9 A student looks at the formula for calcium sulfide, CaS, and makes the following comments:
- **I** Since the ratio of calcium to sulfur in this formula is 1:1, the mass of sulfur required to react with 100 g of calcium will be 100 g.
- **II** 125 atoms of calcium will react exactly with 125 atoms of sulfur.
- **III** The reaction of 5 mol of Ca and 5 mol of S will produce 10 mol of CaS.
- **a** Is comment I correct? Justify your answer.
- **b** Is comment II correct? Justify your answer.
- **c** Is comment III correct? Justify your answer.

10 The ^{12}C isotope is the standard used for comparing element masses.

For ^{12}C, what is its:
- **a** atomic mass
- **b** relative isotopic mass
- **c** molar mass

11 Write balanced equations, including state symbols if required, for the following reactions.
- **a** Methane gas reacts with oxygen gas to produce carbon dioxide gas and water vapour.
- **b** Iron metal reacts with oxygen to form solid iron(III) oxide.
- **c** Zinc hydroxide powder reacts with phosphoric acid (H_3PO_4) solution to produce the precipitate zinc phosphate and water.

12 Explain why the actual yield of a chemical reaction is less than would be predicted from the balanced equation.

Analyse

13 Which of the following compounds has the highest percentage mass of sulfur?

A SO_2
B SO_3
C H_2S
D PbS_2

14 1.5 mol of a substance has a mass of 48 g. The substance is:

A H_2O
B O_2
C NH_3
D CO_2

15 When a sample of palladium is placed in a mass spectrometer, the following peaks are recorded as the isotopic masses and corresponding percentage abundances given in the table below.

Relative isotopic mass	Abundance (%)
101.9049	0.9600
103.9036	10.97
104.9046	22.23
105.9032	27.33
107.9039	26.71
109.9044	11.80

Which isotope will make the largest contribution to the relative atomic mass?

A isotope with isotopic mass 101.9049
B isotope with isotopic mass 105.9032
C isotope with isotopic mass 107.9039
D isotope with isotopic mass 109.9044

16 The table below gives isotopic composition data for argon and potassium.

Element	Atomic number	Atomic mass (amu)	Relative abundance (%)
argon	18	35.978	0.307
		37.974	0.060
		39.974	99.633
potassium	19	38.975	93.3
		39.976	0.011
		40.974	6.69

a Argon has three isotopes but the relative atomic mass is very close to the mass of the heaviest isotope. Explain why.

b Explain why the relative atomic mass of argon is greater than that of potassium, even though potassium has a higher atomic number.

17 For each of the following numbers of molecules, calculate the number of moles of the following quantities.

a 4.50×10^{23} molecules of water (H_2O)
b 9.00×10^{24} molecules of methane (CH_4)
c 2.3×10^{28} molecules of chlorine (Cl_2)
d 1 molecule of sucrose ($C_{12}H_{22}O_{11}$)

18 For each of the following amounts of molecular substances, calculate the:

i number of molecules
ii total number of atoms

a 1.45 mol of ammonia (NH_3)
b 0.576 mol of hydrogen sulfide (H_2S)
c 0.0153 mol of hydrogen nitrate (HNO_3)

19 Calculate the mass of each of the following.

a 0.060 mol of ethane (C_2H_6)
b 0.32 mol of glucose ($C_6H_{12}O_6$)
c 6.8×10^{-3} mol of urea ($(NH_2)_2CO$)
d 6.12 mol of copper atoms (Cu)

20 Calculate the number of moles for each of the following.

a carbon atoms in 1.201 g carbon
b sulfur molecules (S_8) in 10.0 g sulfur
c methane molecules (CH_4) in 20.0 g methane
d aspirin molecules ($C_6H_4(OCOCH_3)COOH$) in 3.00×10^2 mg aspirin

21 For each of the following molecular substances, calculate the:

i number of moles of the substance
ii number of molecules
iii total number of atoms

a 4.2 g of phosphorus (P_4)
b 75.0 g of sulfur (S_8)
c 0.32 g of hydrogen chloride (HCl)

22 Calculate the mass of iron (Fe) that would contain as many iron atoms as there are molecules in 20.0 g water (H_2O).

23 If 6.02×10^{22} molecules of a substance have a mass of 10 g, calculate the molar mass of the substance.

24 Sulfur trioxide gas has a molecular formula of SO_3. A sample of sulfur trioxide contains 1.50×10^{24} molecules of SO_3.

For this sample, determine:

a the number of moles of SO_3
b the number of moles of atoms
c the mass of the sample
d the mass of sulfur in the sample

25 Calculate the molar mass of a substance if:
- **a** 2.00 mol of the substance has a mass of 80.0 g
- **b** 0.10 mol of the substance has a mass of 9.8 g
- **c** 1.7 mol of the substance has a mass of 74.8 g
- **d** 3.50 mol of the substance has a mass of 371 g

26 A new antibiotic has been isolated and only 2.0 mg is available. The molar mass is found to be 12.5 kg mol^{-1}.
- **a** Express the molar mass in g mol^{-1}.
- **b** Calculate the number of moles of antibiotic.
- **c** Determine how many molecules of antibiotic have been isolated.

27 Determine the percentage by mass of carbon in the following substances.
- **a** naphthalene ($C_{10}H_8$)
- **b** ethanoic acid (CH_3COOH)
- **c** urea (NH_2CONH_2)
- **d** aspirin ($C_6H_4(OCOCH_3)COOH$)

28 Determine the empirical formulas of the compounds with the following compositions.
- **a** 27.2% carbon, 72.8% oxygen
- **b** 54.5% carbon, 9.1% hydrogen, 36.4% oxygen
- **c** 9.6 g carbon, 0.67 g hydrogen, 4.7 g chlorine
- **d** 4.42 g carbon, 0.842 g hydrogen

29 A clear liquid extracted from fermented lemons was found to consist of carbon, hydrogen and oxygen. Analysis showed it to be 52.2% carbon and 34.8% oxygen.
- **a** Find the empirical formula of the substance.
- **b** If 2.17 mol of the compound has a mass of 100 g, find the molecular formula of the compound.

30 Find the relative atomic mass of nickel if 3.370 g nickel was obtained by reduction of 4.286 g of the oxide (NiO).

31 A 3.72 g sample of element X exactly reacts with 4.80 g of oxygen to form a compound whose molecular formula is shown, from other experiments, to be X_4O_{10}. Determine the relative atomic mass of X.

32 The equation for the reaction between aluminium metal and oxygen gas is:

$4Al(s) + 3O_2(g) \rightarrow 2Al_2O_3(s)$
- **a** 1.2 mol of aluminium is completely reacted with oxygen gas. Calculate:
  - **i** the number of moles of oxygen gas required for the reaction
  - **ii** the number of moles of aluminium oxide formed
- **b** A reaction produces 0.38 mol of aluminium oxide. Calculate:
  - **i** the number of moles of aluminium that reacted
  - **ii** the number of moles of oxygen gas that reacted

33 When solutions of iron(II) sulfate and potassium hydroxide are mixed, the reaction that occurs can be represented as:

$FeSO_4(aq) + 2KOH(aq) \rightarrow Fe(OH)_2(s) + K_2SO_4(aq)$

Complete the following expressions based on this equation. The first one has been done for you.

$$n(KOH) = \frac{2}{1} \times n(Fe(OH)_2)$$
- **a** $n(FeSO_4) = \frac{\Omega}{\Omega} \times n(KOH)$
- **b** $n(KOH) = \frac{\Omega}{\Omega} \times n(K_2SO_4)$
- **c** $n(Fe(OH)_2) = \frac{\Omega}{\Omega} \times n(FeSO_4)$

34 Carbon disulfide is prepared by reacting coke with excess sulfur dioxide. The balanced equation for this reaction is:

$5C(s) + 2SO_2(g) \rightarrow CS_2(l) + 4CO(g)$

Determine how many grams of carbon monoxide will be produced if 200.0 g of carbon reacts with excess sulfur dioxide.

35 In three separate experiments, different amounts of carbon and oxygen were reacted to produce carbon dioxide, according to the equation:

$C(s) + O_2(g) \rightarrow CO_2(g)$

The table lists the amount of reactants in each of the three experiments. Complete the table to indicate the amount of product formed and the remaining reactant at the end of the reaction.

Carbon atoms available	Oxygen molecules available	Carbon dioxide molecules produced	Carbon atoms in excess	Oxygen molecules in excess
8	20			
1000	3000			
9 mol	6 mol			

36 Sodium can react with oxygen gas to form sodium oxide. The equation for this reaction is:

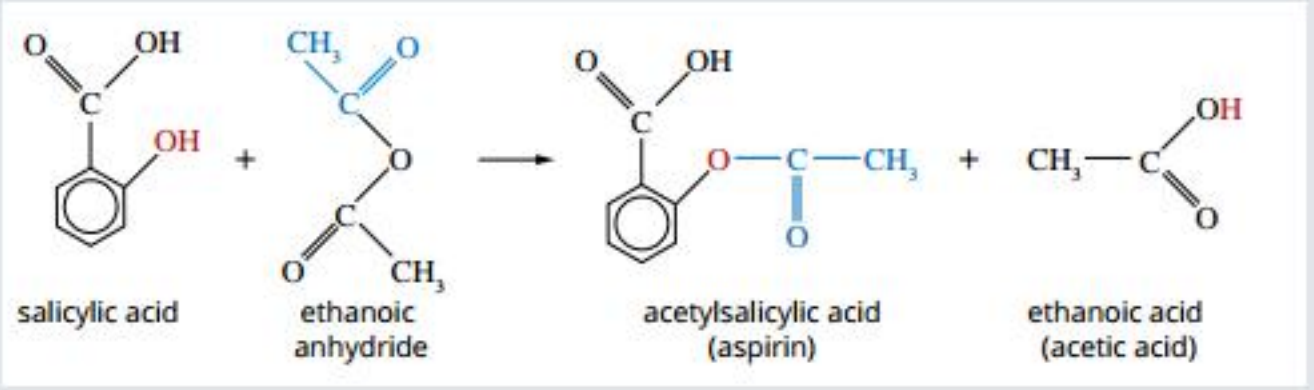
$4Na(s) + O_2(g) \rightarrow 2Na_2O(s)$

A 3.0 mol sample of sodium is reacted with 0.80 mol of oxygen gas.
- **a** Determine which reactant is in excess.
- **b** Determine how many moles of sodium oxide are produced in the reaction.

37 When 4.40 g of P_4O_6 is mixed with 3.00 g of I_2, they react according to this equation:

$5P_4O_6(s) + 8I_2(g) \rightarrow 4P_2I_4(s) + 3P_4O_{10}(s)$
- **a** Determine which reactant is in excess and by how much, in g.
- **b** Determine the mass of P_2I_4 formed.
- **c** Determine the mass of P_4O_{10} formed.
- **d** Determine the total mass of all the products. (Hint: compare this with the mass of the reactants.)

38 Aspirin can be synthesised by an esterification reaction according to the pathway shown below.



A student reacted a 2.50 g sample of salicylic acid with an excess of ethanoic anhydride, using sulfuric acid as a catalyst. After purification, a mass of 2.35 g of pure aspirin was obtained.

a Calculate the theoretical yield of aspirin for the reaction.

b Calculate the percentage yield of aspirin for the reaction.

39 A chemist wishing to manufacture chloroethane reacts a sample of ethane, C_2H_6, with chlorine gas. The equation for the reaction is:

$C_2H_6(g) + Cl_2(g) \rightarrow C_2H_5Cl(g) + HCl(g)$

The mass of ethane used is 3.10 g and the mass of chloroethane obtained is 3.25 g.

a The mass of chloroethane obtained is greater than the mass of ethane used. Does this mean the yield in the reaction is over 100%? Explain your answer.

b Determine the percentage yield of the reaction.

Interpret

40 The chloroethane (C_2H_5Cl) in Question **38** can also be produced from the reaction between ethene gas, C_2H_4, and hydrogen chloride gas, HCl.

The mass of chloroethane formed in a particular reaction was 2.80 g.

a Write an equation for the reaction, knowing chloroethane is the sole product formed.

b Assuming a percentage yield of 100%, determine the mass of ethene that reacted.

c Use the law of conservation of mass to determine the mass of the other reactant, hydrochloric acid.

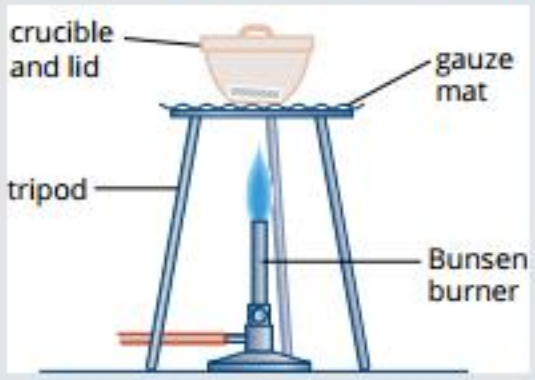
d Answer the following questions:

i Use the mole ratio between ethene and hydrochloric acid to determine the number of moles of hydrochloric acid in the reaction.

ii Calculate the mass of this hydrochloric acid.

ii How does this mass compare to the mass calculated in part **c**?

41 The empirical formula of a metal oxide can be found by experimentation using this equipment.



The mass of the oxygen that reacts with the mass of the metal must be determined. Steps A–F form the experimental method.

a Sort the steps in the correct order by letter.

A Ignite a burner and heat the metal.

B Allow the crucible to cool, then weigh it.

C Continue the reaction until no further change occurs.

D Clean a piece of metal with emery paper to remove any oxide layer.

E Place the metal in a clean, weighed crucible and cover with a lid.

F Weigh the metal and record its mass.

b Two students collected the following data:
mass of the metal = 0.542 g
mass of the empty crucible = 20.310 g
mass of the crucible and metal oxide = 21.068 g
They found from this data that the metal oxide had a 1:1 formula, i.e. MO, where M = metal. Copy and complete the table below, using the data given.

	Metal	**Oxygen**
mass (g)		
relative atomic mass		16.0
moles		
ratio		

c Determine the metal that was used in the experiment.

Data analysis

DATA SET 1

The information below applies to Questions 1–4.

Iron reacts vigorously with chlorine gas. An experiment is conducted to determine the empirical formula of the compound formed. The steps in the experiment are:

1. The mass of a glass tube is recorded.
2. A sample of powdered iron is added to the glass tube and the combined mass of the iron and the tube is recorded.
3. A stream of chlorine gas is passed over the iron sample.
4. The glass tube and the iron in it are heated strongly.
5. Heating and chlorine flow are stopped and the tube is allowed to cool.
6. The tube and contents are weighed and the mass recorded.

The following measurements were obtained:

mass of tube:	86.434 g
mass of tube and iron:	87.564 g
mass of tube and product:	89.704 g

Question 1 (5 marks)

a Determine the mass of iron used in the reaction. (1 mark)

b Determine the mass of chlorine that reacted. (1 mark)

c Use the masses of iron and chlorine to determine the empirical formula of this compound. (3 marks)

Question 2 (2 marks)

Explain how the time the iron is heated for might be an important factor in obtaining accurate results in this procedure.

Question 3 (2 marks)

Write a balanced equation for the reaction that has occurred.

Question 4 (3 marks)

A 1.00 kg sample of this compound is prepared. Determine the masses of iron and chlorine in this sample.

CHAPTER

10 Energy changes in chemical reactions

In Chapter 9, you learnt that chemical reactions involve the rearrangement of atoms to produce new substances, but the total amount of matter remained the same. Matter is not created or destroyed when a chemical change occurs. This law, known as the law of conservation of mass, is fundamental to our understanding of the material universe. But there is a second law that all chemical reactions must obey. This is the law of conservation of energy, and it underpins the concepts you will cover in this chapter.

In this chapter, you will explore the role that energy, in particular heat energy, plays in chemical change. You will learn that all chemical reactions involve changes in energy, and these changes can be calculated and experimentally measured.

Syllabus subject matter

Topic 3 • Chemical reactions—reactants, products and energy change

■ CHEMICAL REACTIONS

- Identify that chemical reactions and phase changes involve energy changes, commonly observable as changes in the temperature of the surroundings and/or the emission of light. **10.1**

■ EXOTHERMIC AND ENDOTHERMIC REACTIONS

- State that heat is a form of energy, and that temperature is a measure of the average kinetic energy of the particles. **10.1**
- Explain how endothermic and exothermic reactions relate to the law of conservation of energy and the breaking and reforming of bonds. **10.2**
- Discriminate between exothermic and endothermic reactions. **10.2**
- Sketch enthalpy level diagrams for exothermic and endothermic reactions. **10.2**
- Analyse enthalpy level diagrams and thermochemical equations to determine the relative stabilities of reactants and products, and the sign of the enthalpy change (ΔH) for a reaction. **10.2**
- Explain, in terms of average bond enthalpies, why reactions are exothermic or endothermic. **10.2**
- Identify the limitations of using average bond enthalpies to calculate enthalpy change. **10.2**
- Calculate the heat change (Q) for a substance given the mass, specific heat capacity and temperature change. (Formula: $Q = mc\Delta T$) **10.3**
- Calculate the enthalpy change (ΔH) for a reaction given temperature changes, quantities of reactants and mass of water. (Formula: $\Delta H = H_{(products)} - H_{(reactants)}$) **10.3**
- Analyse data for heat of combustion, heat of neutralisation and reactions in aqueous solutions to determine heat, mass, specific heat capacity, temperature and enthalpy change. **10.3**

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10.1 Energy change

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the concept of energy and know that the SI unit for energy is the joule
- compare the concepts of system and surrounds
- state that heat is a form of energy and that temperature is a measure of the average kinetic energy of particles
- identify that chemical changes and phase changes involve energy changes
- describe and name the phase changes: melting, freezing, vaporisation, condensation, sublimation and deposition.

Before the invention of agriculture, a person in an early hunter–gatherer society used approximately 10 MJ of energy per day. Despite being less active than hunter–gatherers, a person in our modern industrial society uses, on average, nearly 1000 MJ per day. This figure is 100 times greater than the body's basic requirement. The bulk of the energy used, directly or indirectly, comes from the combustion of fuels such as coal, natural gas or petrol. Coal is burnt in coal-fired power stations, like the one in Figure 10.1.1, where the heat released is used to generate electricity. Some activities use small amounts of energy, whereas others such as launching a space shuttle (Figure 10.1.2), use enormous amounts of energy.

FIGURE 10.1.2 The space shuttle *Endeavour* taking off from Kennedy Space Center in Cape Canaveral, Florida. The solid rocket boosters, which helped propel the shuttle into space, consumed 5000 kg of fuel per second, releasing the same amount of energy as 14 700 diesel-powered locomotives.

FIGURE 10.1.1 There are several coal-fired power stations in Queensland, like this one near Gladstone, which generate electricity by burning coal. The heat comes from the combustion of the coal, which powers turbines to generate electricity.

In this module, you will define what energy is, and the role it plays in chemical reactions and physical changes. You will look specifically at heat and temperature, and see how these concepts help us to understand changes of state.

CHEMICAL ENERGY

Chemical reactions occur when particles (atoms, molecules or ions) collide and are rearranged to form new particles. All chemical reactions involve energy changes. Unlike matter, you know the effects of energy without being able to directly see, touch, smell or weigh it. **Energy** is usually defined as the capacity to do work, that is, the capacity to move an object against an opposing force. It comes in many forms, and includes heat, light, sound, electricity and chemical energy.

Chemical energy is the energy stored in the bonds between the atoms and molecules of a substance. It results from factors such as the attractions between electrons and protons in atoms, repulsions between nuclei, repulsions between electrons, movement of electrons, and the vibration and rotations around bonds.

During a chemical reaction, a **reactant** substance is transformed into a **product** substance. This new substance may have a different amount of chemical energy stored in its bonds, so the reaction will either absorb or release energy as it progresses from reactants to products. For example when you eat a meal (Figure 10.1.3), the bonds within the food molecules have stored energy that your cells can access to provide energy for other chemical and physical activities that take place in your body. When wood in Figure 10.1.4 is burned the chemical energy stored in the chemical bonds is released as heat and light. The study of energy changes that occur during chemical reactions is called **thermochemistry**.

The SI (International System of Units) unit for energy is the **joule**, J. Other units also used for quantifying energy are kilojoules, kJ, and megajoules, MJ.

The relationship between joules, kilojoules and megajoules is:

$$1\,J = 10^{-3}\,kJ = 10^{-6}\,MJ$$

This can also be expressed as:

$$1\,MJ = 1000\,kJ = 1\,000\,000\,J$$

Figure 10.1.5 shows how you can convert between different units of energy.

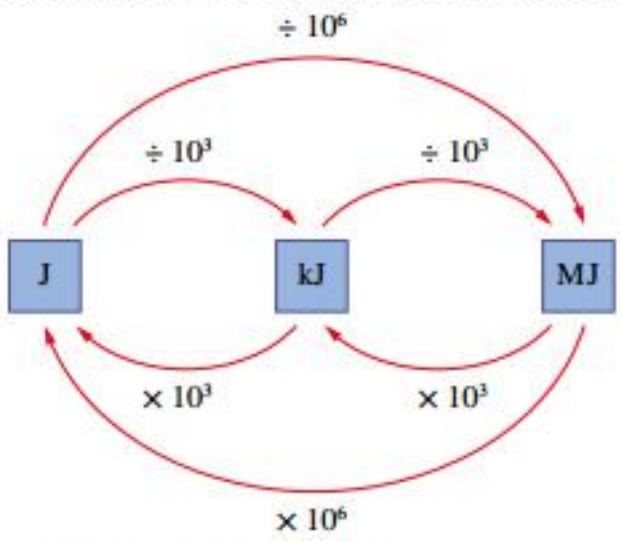


FIGURE 10.1.5 Converting between different energy units.

Chemical energy is the energy stored in the bonds between the atoms and molecules of a substance.

FIGURE 10.1.3 When you eat food, you access the chemical energy stored in the food. This energy powers all of the chemical reactions and physical activities that take place in your body.

FIGURE 10.1.4 The combustion of wood in a fire releases energy in the form of heat and light.

SYSTEMS AND SURROUNDINGS

Energy changes in chemical reactions often refer to a **system** and its **surroundings**. In chemistry, the system is usually the chemical reaction. When energy is released or absorbed by a system, it means that energy changes occur as bonds are broken and formed between the atoms of the elements involved in the reaction.

The surroundings are usually regarded as everything else. For example, the walls of a container in which a reaction takes place in the gas phase, or the water in a solution in which a reaction takes place in the aqueous phase, can be regarded as the surroundings for the reaction. Energy leaves the system (the reaction) and enters the surroundings, or leaves the surroundings and enters the system.

HEAT AND TEMPERATURE

The reactants in a chemical reaction have a certain amount of chemical energy stored in their bonds. The products that form as a result of the rearrangement of particles during the chemical reaction have different bonds and so have a different amount of chemical energy. Energy will be released or absorbed during the reaction depending on the relative energies of the bonds within the reactants and products. When **fuels**, for example, undergo **combustion**, they release energy that can be used. This is what makes them fuels.

A fuel is a substance that can release stored energy relatively easily. A combustion reaction is a reaction in which a substance (usually a **hydrocarbon**) reacts with oxygen gas, releasing energy, carbon dioxide and water.

Heat (Q) is the energy that flows from one object to another because of a difference in temperature.

Often the energy released to or absorbed from the surroundings is in the form of **heat** (thermal energy). Heat is represented with the symbol q, and is defined as the energy that flows from one object to another because of a difference in **temperature**. If you add heat to an object you will increase its temperature, and heat flows spontaneously from warmer objects to cooler objects. If two objects remain in contact, heat will flow until the two objects are the same temperature.

While heat is the flow of energy, temperature is a measure of the average kinetic energy of the particles of an object. If the same amount of heat energy flows into two different objects, the temperature change will not be the same. One object may be smaller, with less particles, so it would experience a larger temperature increase (Figure 10.1.6). The increase in temperature of an object depends on the mass of the object, the amount of heat added, and the nature of the substance. Different substances, with different types of bonds between their atoms and molecules, have differing capacities to absorb heat.

FIGURE 10.1.6 The water in the kettle in (a) has a higher temperature but the water in the swimming pool in (b) has more heat energy. It would take more heat to raise the temperature of the swimming pool by 1°C than the kettle because there are more water molecules in the swimming pool.

Temperature is a measure of the average kinetic energy of the particles that make up an object. Temperature is measured with the Celsius (°C) or Kelvin (K) scale.

Temperature can be measured with a thermometer on the **Celsius** (°C) **scale**, where 0°C is the temperature at which water freezes at a pressure of 101.3 kPa. In chemistry, temperature is often measured on the **Kelvin scale** (K). The Kelvin scale is named after Lord Kelvin (Figure 10.1.7) who proposed the scale in 1848. Zero on the Kelvin scale is the temperature at which particles have no energy, and is equivalent to −273°C. Temperatures can be converted from Celsius to the Kelvin scale by the relationship:

$$T(\text{K}) = T(^\circ\text{C}) + 273$$

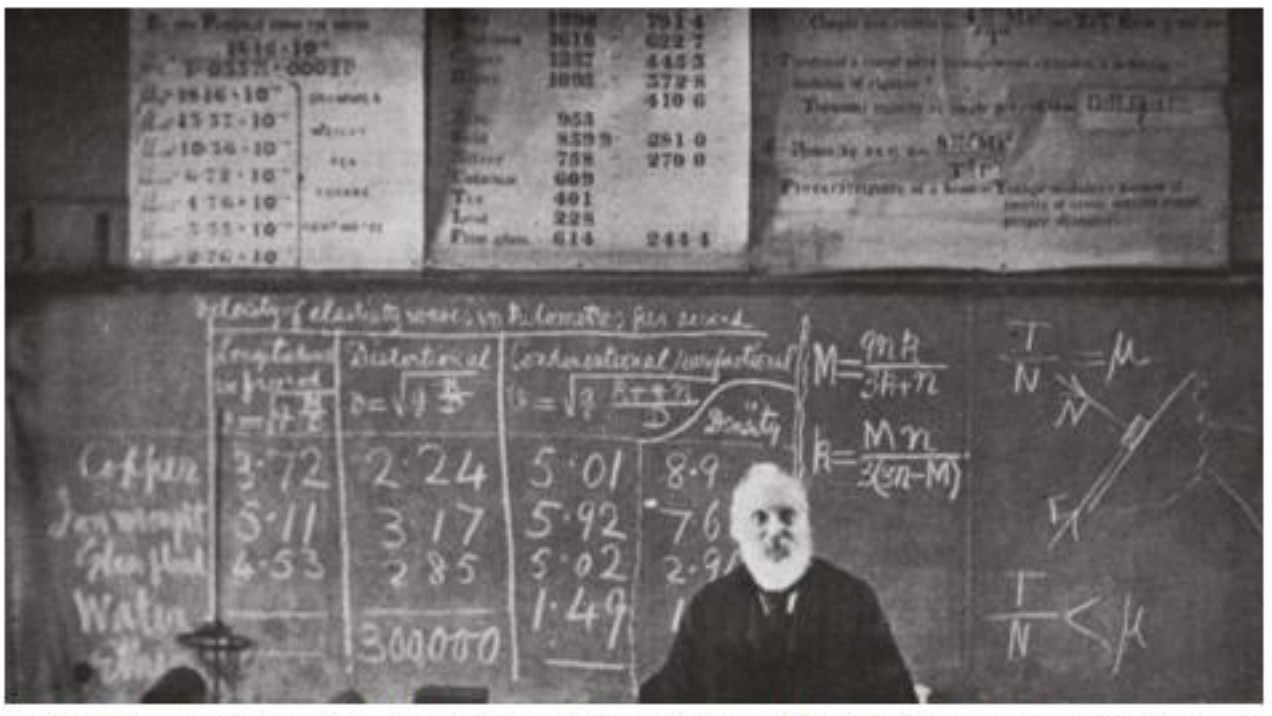


FIGURE 10.1.7 Kelvin (1824–1907) proposed the existence of absolute zero in 1848 and the use of an absolute temperature scale.

One degree Celsius is equal to one kelvin, so when changes in temperature are measured, they can equally be expressed in degrees C or K.

$$1°C = 1\,K$$

STATES OF MATTER

If you consider the example of the chemical water (H_2O), three different words can be used to describe it—water, ice or steam. Imagine if somebody dropped a 25 kg block of ice on your head. It would have a very different effect to dropping 25 kg of water on your head! Methane, like most substances, can also exist in three different physical **states** (or **phases**) **of matter**, which are: solid, liquid and gas (Figure 10.1.8). Changes of state, such as a solid melting to form a liquid, are a type of physical change, rather than a chemical change. These changes also involve energy being absorbed or released.

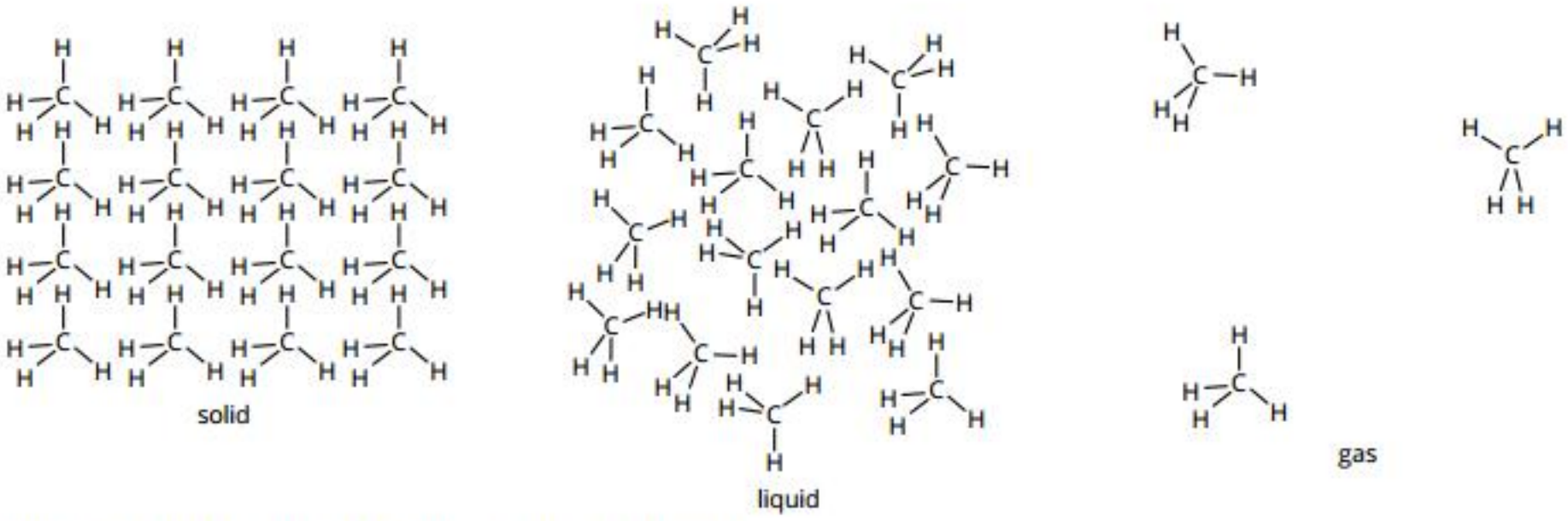


FIGURE 10.1.8 The chemical methane (CH_4) can exist as a solid, liquid or gas.

Matter in a **solid** state has a definite shape and volume, and the shape does not depend on the shape of the container. The particles in a solid are packed tightly together, often in an orderly arrangement. Due to the arrangement of their particles, solids are effectively incompressible.

Matter in a **liquid** state does not have a defined shape, and will take the shape of the container it is placed in. The particles in a liquid are in close contact with one another, but the arrangement is not fixed or orderly. The particles are free to move from one location to another, but the volume is fixed and like solids, liquids are almost incompressible.

Matter in a **gaseous** state takes the shape and volume of its container. This is because the particles in gases are no longer in contact with one another and are free to move. Compared to solids and liquids, the particles in a **gas** are much further apart, so gases are much more easily compressed. Sometimes the word **vapour** is used interchangeably with the word 'gas'.

Kinetic theory explains the differences in the physical properties of the different states of matter. Kinetic theory states that all matter consists of particles in motion, and as the temperature increases the movement of the particles increases. Most substances can exist in all three states, and the state at a given temperature and pressure is determined by the strength of the inter-particle forces.

There are three states of matter, which can be characterised in terms of the arrangement and movement of the particles and the forces between them: solid, liquid and gas.

Kinetic theory states that all matter consists of particles in motion, and as the temperature increases, the movement of the particles increases.

Heat flow results from the microscopic movement and collisions of particles (Figure 10.1.9). When heat moves between two systems at different temperatures, the kinetic energy of the warmer system's particles is transferred to the cooler system's particles. When the temperature increases enough, and the particles have sufficient energy to overcome inter-particle forces, a **change of state** occurs. When the vibrations of the particles of a solid have sufficient energy, they will move away from their fixed positions and take liquid form. This process is called **melting**, and the reverse process (liquid to solid) is called **freezing**. If the particles of a substance in a liquid state absorb enough energy, some may have sufficient energy to break away from the surface of the liquid. These particles are said to **evaporate** (Figure 10.1.10). When there is sufficient energy for all the particles to break apart, the substance is said to have reached **boiling point**. **Evaporation** and boiling are both types of **vaporisation**. The reverse of vaporisation (gas to liquid) is **condensation**.

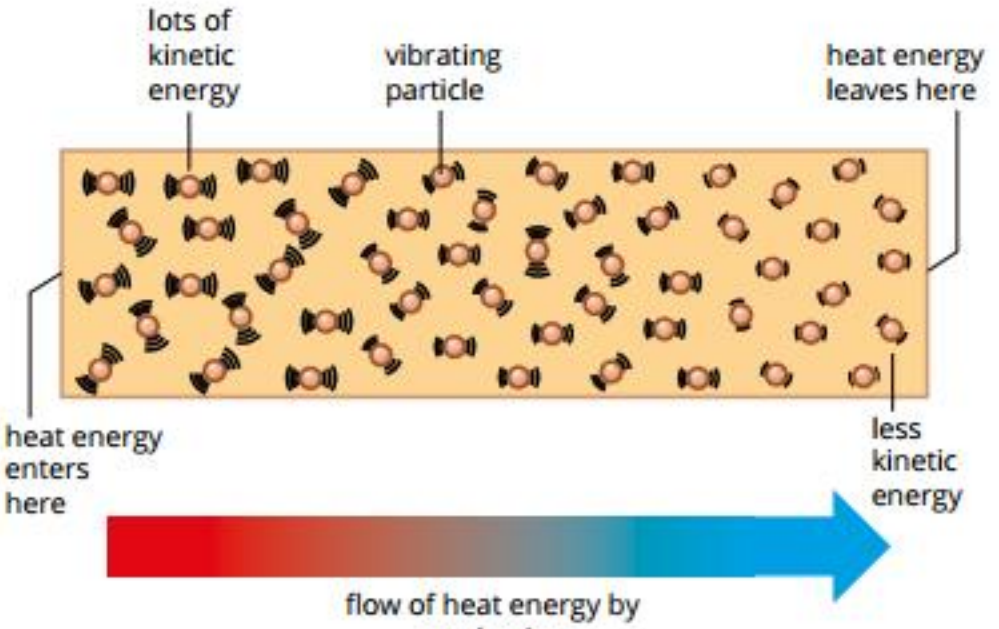


FIGURE 10.1.9 Heat flow, in this case by conduction, results from the microscopic movement and collisions of particles.

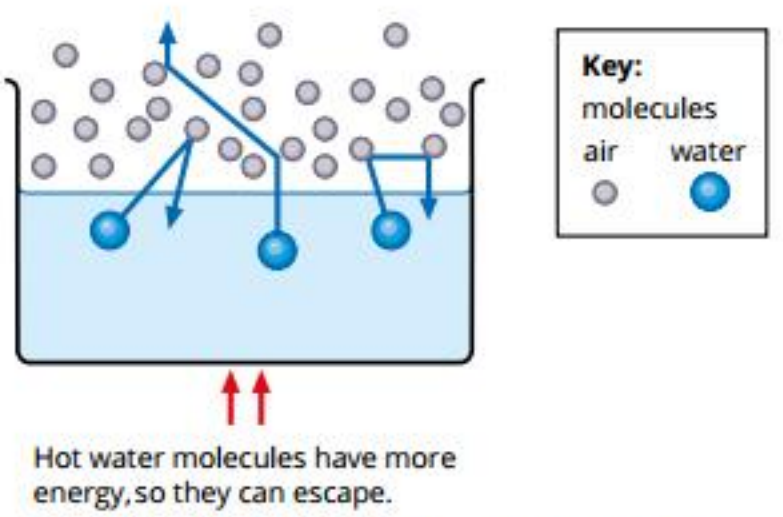


FIGURE 10.1.10 When water molecules have enough heat energy to overcome inter-particle forces, they will break away from the liquid. This process is called evaporation.

FIGURE 10.1.11 Dry ice, or carbon dioxide (CO_2) in its solid state, will sublime at room temperature.

It is possible, under certain temperatures and pressures, for solids to go directly to a gaseous state without passing through an intermediate liquid state. This type of state change is known as **sublimation**. In Figure 10.1.11, solid carbon dioxide (CO_2), or dry ice, is sublimating at room temperature. The reverse of sublimation is **deposition**. Figure 10.1.12 summarises the different changes of state.

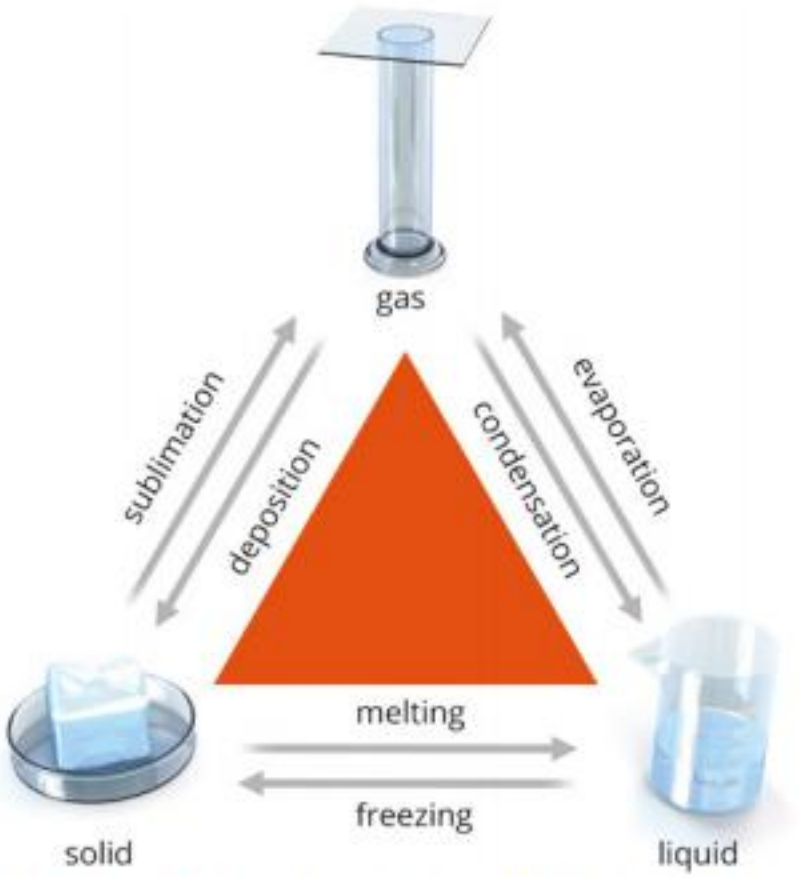


FIGURE 10.1.12 A summary of the possible state changes that can occur between solid, liquid and gas.

Consider the heating curve for water below in Figure 10.1.13.You will notice that while the water is undergoing a change of state the temperature does not increase. This is because the heat energy being absorbed by the substance is being used to break the **intermolecular bonds** (the bonds between molecules). As a result, the average kinetic energy or temperature of the substance does not increase. Once all the particles have changed state, and the intermolecular bonds have been overcome, the temperature starts increasing again.

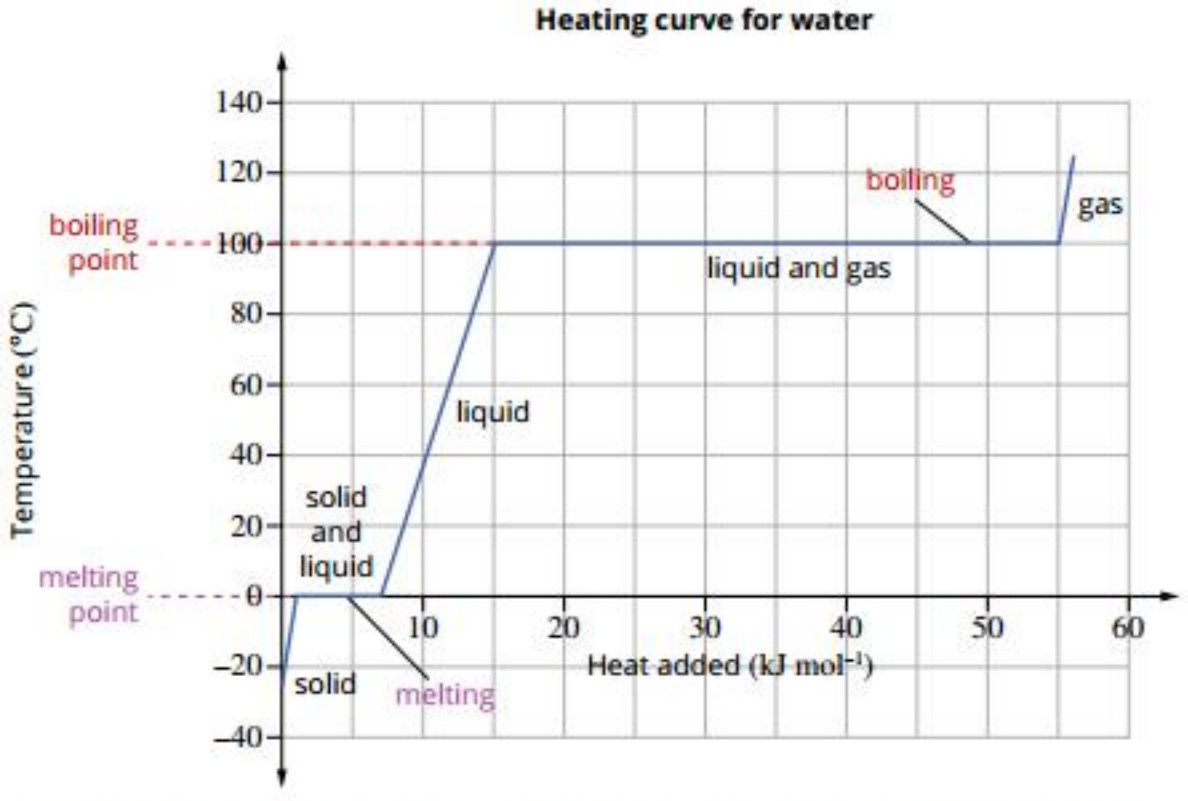


FIGURE 10.1.13 The heating curve for water. While the water is undergoing a change of state the temperature does not increase. Notice the state change from liquid to gas needs more energy than solid to liquid as the intermolecular bonds are broken during this process.

10.1 Review

SUMMARY

- Chemical energy is the energy stored in the bonds between the atoms and molecules of a substance. The SI unit for energy is the joule, J.
- All chemical reactions involve a change in energy due to the breaking of reactant bonds and the formation of new bonds.
- The system is the chemical reaction and the surroundings are everything else.
- Heat (q), is defined as the energy that flows from one object to another because of a difference in temperature.
- Temperature is a measure of the average kinetic energy of the particles of an object. Temperature is measured on the Celsius (°C) or Kelvin (K) scale.
- Kinetic theory states that all matter consists of particles in motion, and as the temperature increases, the movement of the particles increases.
- Matter can exist in three different physical states (or phases): solid, liquid and gas.
- When the temperature increases enough for the particles to have sufficient energy to overcome inter-particle forces, a change of state occurs.

KEY QUESTIONS

Describe

1 Define chemical energy.

2 State the symbol used to represent heat.

3 Select one term from the following list to replace each phrase describing a change of state:
melting; freezing; evaporation; condensation; boiling point; vaporisation; sublimation; deposition.

a a state change in which a solid passes directly to a gaseous state

b when particles in a liquid state have sufficient energy to break away from the surface of the liquid

c the reverse change of state from condensation

d the change of state in which a liquid loses energy and the particles take on an orderly arrangement

Apply

4 Explain the difference between the terms 'system' and 'surroundings' in relation to a chemical reaction.

5 A student reacts an aqueous solution of an acid and an aqueous solution of a base together in a beaker. Describe the system in this scenario.

6 A sample of gas in a sealed container of fixed volume is heated. Use the kinetic theory to predict what will happen to the average speed of the gas particles.

7 Convert the following Celsius temperatures to absolute temperatures in K.

a 25.0°C

b −183.2°C

c 1450°C

d −272.8°C

8 Convert the following absolute temperatures to temperatures in °C.

a 45 K

b 199.2 K

c 312 K

d 455.5 K

Analyse

9 Explain the three states of matter in terms of kinetic theory.

10 Convert the following energy values to kilojoules (kJ).

a 0.180 MJ

b 1.5×10^6 J

c 10.0 J

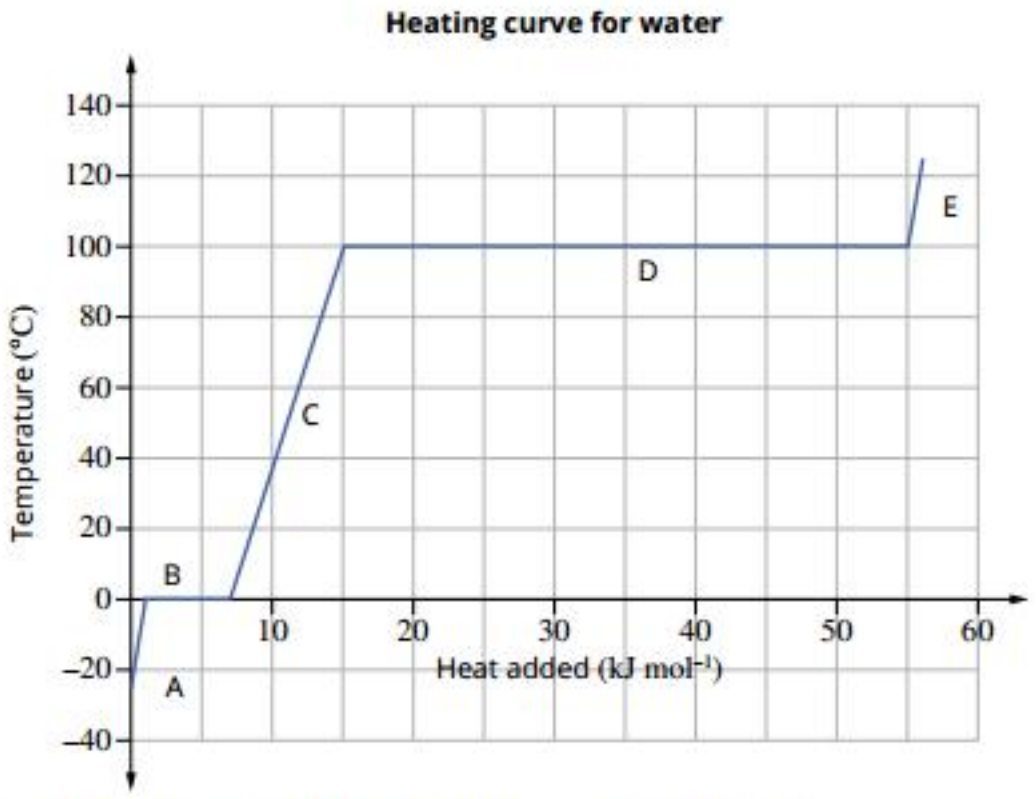
d 2.0×10^{-3} J

11 Explain the difference between heat and temperature.

12 Consider the heating curve for water depicted in Figure 10.1.13 on page 219. Explain why the temperature does not rise when the water begins to boil.

13 What is the difference between the Celsius and Kelvin temperature scales?

14 The following graph plots temperature against time as a sample of water is heated.



Match one of the letters to each statement below. Each letter may be used more than once.

a Molecules have the greatest kinetic energy.
b State change from solid to liquid.
c Liquid water being heated in a saucepan.
d Both ice and liquid water present.
e All the intermolecular bonds have been overcome.
f The water in the saucepan is boiling.

10.2 Exothermic and endothermic reactions

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- explain the law of conservation of energy and explain how it relates to endothermic and exothermic reactions
- discriminate between exothermic reactions and endothermic reactions in terms of energy change
- understand the concept of enthalpy
- write thermochemical equations and use them to perform calculations using average bond enthalpies
- use average bond enthalpy to explain whether a reaction is exothermic or endothermic
- identify the limitations of using average bond enthalpies to calculate enthalpy change
- sketch and analyse enthalpy level diagrams.

FIGURE 10.2.1 The reaction between sodium and chlorine gas releases energy into the surroundings.

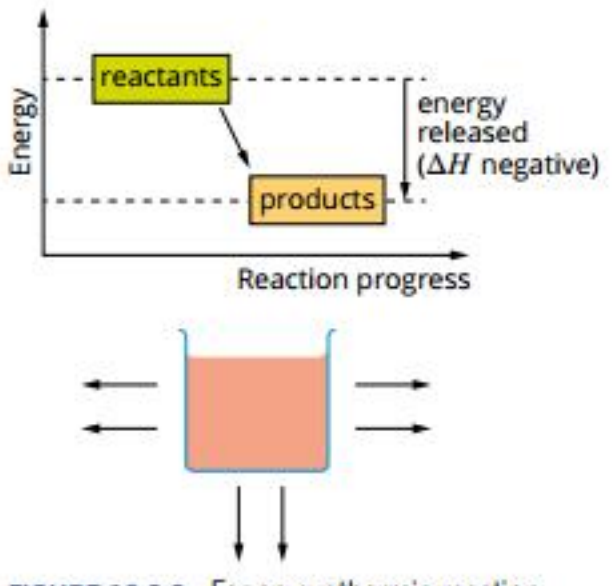


FIGURE 10.2.2 For an exothermic reaction, the enthalpy of the reactants is greater than the enthalpy of the products, so energy is released to the surroundings during the reaction.

Chemical reactions always involve energy changes. As the reactant particles are rearranged, the chemical energy of the reactants will be different to that of the products. In some chemical reactions, for example the combustion of fuels, the rearrangement of atoms causes energy to be released to the surroundings. In other chemical reactions, for example photosynthesis, energy is absorbed from the surroundings as the chemical reaction takes place. The energy change in some reactions is very small and can only be measured with specialised equipment.

In this module, you will learn about the energy changes that occur during chemical reactions. You will also learn how to classify chemical reactions based on their energy changes.

EXOTHERMIC AND ENDOTHERMIC PROCESSES

Whenever a chemical reaction or change in physical state occurs, there is a change in the energy of the system. This energy difference is usually either absorbed from or released to the surroundings as heat. Figure 10.2.1 shows the reaction between sodium and chlorine gas. In this reaction, a change in energy can be seen with the release of heat and light. The **law of conservation of energy** states that during any chemical or physical process, energy is neither created nor destroyed. In thermochemistry, this means that if the energy of the system increases during a chemical reaction, the energy of the surroundings must decrease by the same amount.

When the total chemical energy of the products of a chemical reaction is less than the total chemical energy of the reactants, the excess energy is released to the surroundings. In thermochemical calculations, heat flow is described from the point of view of the system. If energy 'exits' the reaction system then the chemical reaction is called an **exothermic** reaction (Figure 10.2.2). The released energy can be shown in a chemical equation by writing 'energy' on the product side of the arrow.

For example, the production of water from the reaction between hydrogen and oxygen gas is an exothermic reaction. This can be represented by the balanced equation:

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l) + \text{energy}$$

Another example of an exothermic reaction is the combustion of methane gas:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g) + \text{energy}$$

When the total chemical energy of the products of a chemical reaction is greater than the total chemical energy of the reactants, energy is absorbed from the surrounding environment. Energy 'enters' the reaction system and the chemical reaction is called an **endothermic** reaction (Figure 10.2.3). If an endothermic reaction takes place in a container, the container may feel cold to the touch. This is because the reaction system is absorbing heat from the surroundings, leaving the environment, including the container, cooler.

For an endothermic reaction, the energy that is required can be written on the reactant side of the equation arrow. For example, the decomposition of calcium carbonate is an endothermic process. This can be represented by the balanced equation:

$$CaCO_3(s) + \text{energy} \rightarrow CaO(s) + CO_2(g)$$

Endothermic reactions require the constant input of energy.

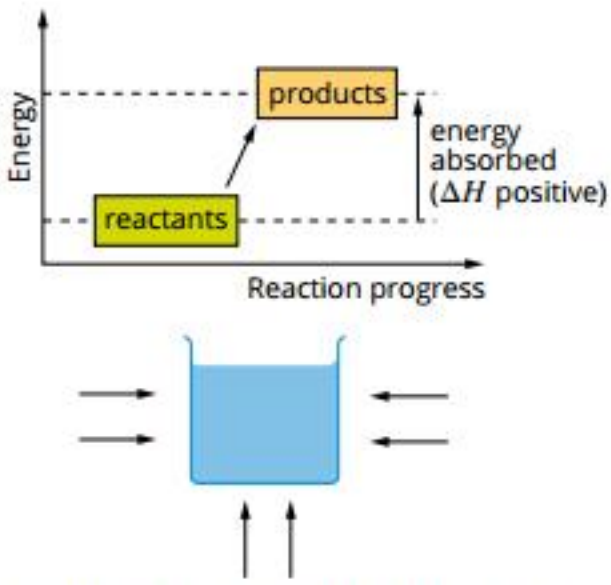


FIGURE 10.2.3 For an endothermic reaction, the enthalpy of the reactants is less than the enthalpy of the products so energy is absorbed during the reaction.

Enthalpy

The chemical energy of a substance is sometimes called its **heat content** or **enthalpy**. It is given the symbol H. The enthalpy of the reactants in a chemical reaction is given the symbol H_r and the enthalpy of the products is given the symbol H_p.

Most chemical processes take place in open systems under a constant pressure (usually atmospheric). The exchange of heat energy between the system and its surroundings under constant pressure is referred to as the **enthalpy change**, or **heat of reaction**, and is given the symbol ΔH. The capital delta symbol (Δ) is commonly used in chemistry to represent 'change in'. For example, ΔT is the symbol for change in temperature.

For the general reaction, reactants → products, the enthalpy change (ΔH) is calculated by:

$$\Delta H = H_{(\text{products})} - H_{(\text{reactants})}$$

When $H_{(\text{products})}$ is less than $H_{(\text{reactants})}$, energy is released from the system into the surroundings, so the reaction is exothermic. The system has lost energy, so ΔH has a negative value. Therefore, for exothermic reactions, $\Delta H < 0$. When H_p is greater than H_r, energy must be absorbed from the surroundings, so the reaction is endothermic. The system has gained energy, so ΔH has a positive value, i.e. $\Delta H > 0$.

If the total chemical energy of the products is less than the total energy of the reactants, energy will be released from the system into the surroundings. This is called an exothermic reaction.

If the total chemical energy of the products is greater than the total energy of the reactants, energy will be absorbed from the surroundings. This is called an endothermic reaction.

THERMOCHEMICAL EQUATIONS

The enthalpy change can be shown by writing the ΔH value to the right of the chemical equation. Such an equation is called a **thermochemical equation**. The ΔH value in a thermochemical equation usually has the units $kJ\,mol^{-1}$. This means that the amount of energy (in kJ) signified by the ΔH value corresponds to the mole amounts specified by the coefficients in the equation.

For example, consider the cellular respiration of glucose:

$$C_6H_{12}O_6(aq) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l) \qquad \Delta H = -2803\,kJ\,mol^{-1}$$

This thermochemical equation tells you that when 1 mole of glucose reacts with 6 moles of oxygen to produce 6 moles of carbon dioxide and 6 moles of water, 2803 kJ of energy is released. The ΔH is negative because the reaction is exothermic.

Enthalpy changes also occur during physical changes, so thermochemical equations can be written for physical changes. Melting ice is an example of a physical change. It is an endothermic process, because heat must be applied to solid ice to convert it into liquid water. The thermochemical equation for this change is:

$$H_2O(s) \rightarrow H_2O(l) \qquad \Delta H = +6\,kJ\,mol^{-1}$$

The ΔH value is positive because the process is endothermic.

Enthalpy change is a measure of the amount of energy absorbed or released during chemical reactions. It is given the symbol ΔH and is determined by subtracting the enthalpy of the reactants from the enthalpy of the products.

For an exothermic reaction, ΔH is negative; for an endothermic reaction, ΔH is positive.

Thermochemical equations and mole ratios

The ΔH value in a thermochemical equation corresponds to the mole amounts specified by the equation. If the coefficients in the equation are changed, the ΔH value will also change.

For example, the balanced thermochemical equation for the combustion of methanol can be written as:

$$CH_3OH(l) + \frac{3}{2}O_2(g) \rightarrow CO_2(g) + 2H_2O(l) \qquad \Delta H = -726\,kJ\,mol^{-1}$$

This means that 726 kJ of energy is released when 1 mole of methanol reacts with 1.5 moles of oxygen gas, to produce 1 mole of carbon dioxide and 2 moles of water. If twice as much methanol were to react, then twice as much energy would be released. So, if the coefficients of the equation are doubled, the enthalpy change of the reaction (ΔH) value is also doubled:

$$2CH_3OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 4H_2O(l) \qquad \Delta H = -1452\,kJ\,mol^{-1}$$

If the mole amounts are tripled, the ΔH value is also tripled:

$$3CH_3OH(l) + \frac{9}{2}O_2(g) \rightarrow 3CO_2(g) + 6H_2O(l) \qquad \Delta H = -2178\,kJ\,mol^{-1}$$

The ΔH value provided adjacent to the reaction is specific for that reaction. We interpret the 'per mole' in the units of ΔH ($kJ\,mol^{-1}$) by noting the stoichiometric coefficients in the chemical equation. In the above case, '$2178\,kJ\,mol^{-1}$' indicates 2178 kJ is produced 'per 3 mole CH_3OH', 'per $\frac{9}{2}$ mole O_2', 'per 3 mole CO_2', and 'per 6 mole H_2O'.

It is important to always include **state symbols** (s, l, g) in thermochemical equations. Physical changes involve an enthalpy change, so the state of the species in a chemical reaction affects the enthalpy change of the reaction. For example, both of the following equations represent physical changes involving water. They have different ΔH values because the states are different.

$$H_2O(s) \rightarrow H_2O(l) \qquad \Delta H = +6\,kJ\,mol^{-1}$$
$$H_2O(l) \rightarrow H_2O(g) \qquad \Delta H = +44\,kJ\,mol^{-1}$$

You can see that it requires more energy to boil water than it does to melt ice.

Reversing a chemical equation changes the sign but not the magnitude of ΔH. For example, methane (CH_4) reacts with oxygen gas to produce carbon dioxide gas and water in an exothermic reaction:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l) \qquad \Delta H = -890\,kJ\,mol^{-1}$$

If this reaction is reversed, the magnitude of ΔH remains the same because the enthalpies of the individual chemicals have not changed, but the sign changes to indicate that energy must be absorbed for this reaction to proceed.

$$CO_2(g) + 2H_2O(l) \rightarrow CH_4(g) + 2O_2(g) \qquad \Delta H = +890\,kJ\,mol^{-1}$$

Worked example 10.2.1

CALCULATING ΔH FOR A REACTION

Iron reacts with oxygen according to the equation:

$$3Fe(s) + 2O_2(g) \rightarrow Fe_3O_4(s) \qquad \Delta H = -1121\,kJ\,mol^{-1}$$

Calculate ΔH for the reaction represented by the equation:

$$2Fe_3O_4(s) \rightarrow 6Fe(s) + 4O_2(g)$$

Thinking	Working
The reaction has been reversed in the second equation, so the sign for ΔH is changed to the opposite sign.	ΔH for the second equation is positive.
Identify how the mole amounts in the equation have changed.	The mole amount of Fe_3O_4 has changed from 1 to 2, O_2 has changed from 2 to 4 and Fe has changed from 3 to 6. They have all doubled.
Identify how the magnitude of ΔH will have changed for the second equation.	The mole amounts of the chemicals have all doubled, so ΔH will also have doubled.

Calculate the new *magnitude* of ΔH. (You will write the sign of ΔH in the next step.)	2×1121 $= 2242$
Write ΔH for the second equation, including the sign.	$\Delta H = +2242\,kJ\,mol^{-1}$

➤ Try yourself 10.2.1

CALCULATING ΔH FOR A REACTION

Carbon reacts with hydrogen according to the equation:

$$6C(s) + 3H_2(g) \rightarrow C_6H_6(g) \qquad \Delta H = +49\,kJ\,mol^{-1}$$

Calculate ΔH for the reaction represented by the equation:

$$3C_6H_6(g) \rightarrow 18C(s) + 9H_2(g)$$

ENTHALPY LEVEL DIAGRAMS

The energy required to break the bonds of reactants so that a reaction can proceed is called the **activation energy**. The activation energy is an energy barrier that must be overcome before a reaction can get started.

An activation energy barrier exists for both exothermic and endothermic reactions. If the activation energy for a reaction is very low, the chemical reaction can be initiated as soon as the reactants come into contact because the reactants already have sufficient energy for a reaction to take place. Once an exothermic reaction has started the energy released is often sufficient to overcome the activation energy and so the reaction continues. An example of this can be seen in the reaction between zinc and hydrochloric acid.

The reaction between zinc and hydrochloric acid produces hydrogen gas:

$$Zn(s) + 2HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$$

As you can see in Figure 10.2.4, bubbles of hydrogen gas are vigorously produced as soon as zinc is added to the acid.

The energy changes that occur during a chemical reaction can be shown on an **enthalpy level diagram**. The enthalpy level diagram for an exothermic combustion reaction, like the one shown in Figure 10.2.5, indicates that the enthalpy of the products is always less than the enthalpy of the reactants. Overall, energy is released and so the ΔH value is negative. The enthalpy level diagram also shows that, even in exothermic reactions, the activation energy must first be absorbed to start the reaction.

The enthalpy level diagram for an endothermic reaction (Figure 10.2.6) shows that the enthalpy of the products is greater than the enthalpy of the reactants. Overall, energy is absorbed and so the ΔH value is positive. The diagram also shows the absorption of the activation energy before the release of energy as bonds form in the products.

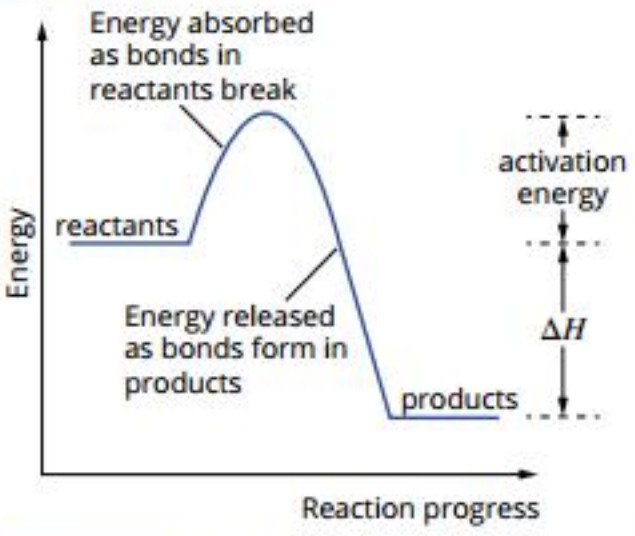


FIGURE 10.2.5 The characteristic shape of an enthalpy level diagram for an exothermic reaction.

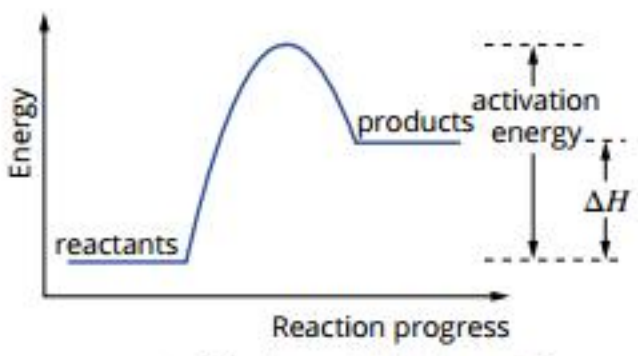


FIGURE 10.2.6 The characteristic shape of an enthalpy level diagram for an endothermic reaction.

ℹ A reaction cannot proceed until the bonds in the reactants are broken. The energy required to do this is the activation energy.

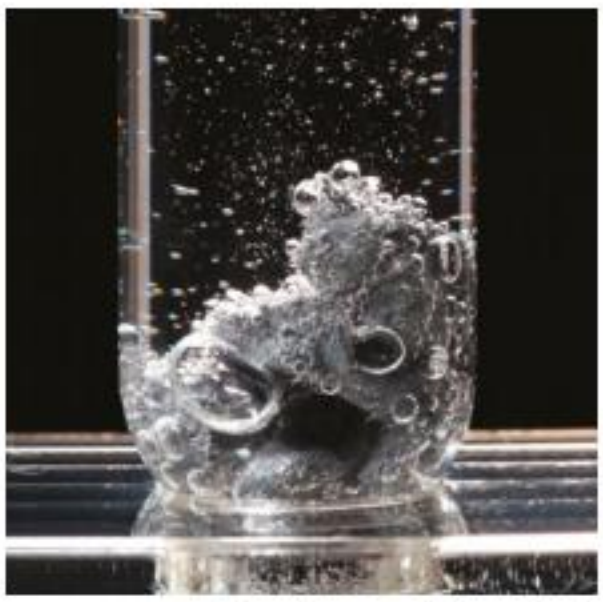


FIGURE 10.2.4 When zinc comes into contact with hydrochloric acid, it reacts almost immediately. The reactants have sufficient energy to 'overcome' the activation energy barrier.

Predicting relative stability

The enthalpy level diagram and the sign (+ve or –ve) of the enthalpy change can be used to predict the comparative stability of the reactant and product chemicals. A reaction is exothermic overall if the bonds that are formed are stronger (higher energy) than the bonds that are broken. A reaction is endothermic when the broken bonds are stronger (higher energy) than the bonds being formed.

BOND ENTHALPIES

Chemical reactions involve making and breaking chemical bonds. The energy changes in a chemical reaction are due to the difference between the energy used to break the reactant bonds and the energy released when new bonds are formed in the products.

> **i** Breaking chemical bonds is an endothermic process, and making chemical bonds is an exothermic process.

An ionic bond is a type of chemical bond that involves the electrostatic attraction between oppositely charged ions. Likewise, a covalent bond is due to the electrostatic attraction between the shared pair of electrons and the positive nuclei of the bonded atoms. Since energy is required to break bonds, the reaction is endothermic.

Forming bonds involves the bringing together of atoms that are attracted by an electrostatic force. Since this is the reverse reaction of breaking bonds, it stands to reason that the formation of bonds releases energy. That is bond formation is exothermic. The same amount of energy is absorbed when a bond is broken as is given out when the bond is made.

The energy needed to break one mole of bonds of gaseous molecules under standard conditions (25°C, 1 atm pressure) is known as the **bond enthalpy**. For example, 436kJ of energy is required to break 1 mole of bonds in hydrogen molecules, forming 2 moles of hydrogen atoms. This process can be written as:

$$H_2(g) \rightarrow 2H(g) \qquad \Delta H = +436\,kJ\,mol^{-1}$$

The bond enthalpies of diatomic molecules can be accurately measured. However, in larger molecules it is often difficult to successively break bonds one at a time to measure bond enthalpies. In these larger molecules, it is usual to quote the **average bond enthalpy**.

Consider the complete dissociation of methane:

$$CH_4(g) \rightarrow C(g) + 4H(g) \qquad \Delta H = +1662\,kJ\,mol^{-1}$$

This is made up of the four processes:

$$CH_4(g) \rightarrow CH_3(g) + H(g) \qquad \Delta H = +435\,kJ\,mol^{-1}$$
$$CH_3(g) \rightarrow CH_2(g) + H(g) \qquad \Delta H = +444\,kJ\,mol^{-1}$$
$$CH_2(g) \rightarrow CH(g) + H(g) \qquad \Delta H = +444\,kJ\,mol^{-1}$$
$$CH(g) \rightarrow C(g) + H(g) \qquad \Delta H = +339\,kJ\,mol^{-1}$$

These equations represent the breaking of a C–H bond. However, they are not all identical because the bond is being broken from a different reactant particle each time.

The average bond enthalpy for the C–H bond could be determined by averaging the above values.

$$\text{Average bond enthalpy for C–H bond} = \frac{+435 + 444 + 444 + 339}{4}$$
$$= \frac{1662}{4}$$
$$= 415.5\,kJ\,mol^{-1}$$

Tables 10.2.1 and 10.2.2 show the average bond enthalpies for various single and multiple bonds. The table values make the assumption that the bond enthalpy is the same in different molecules. As the values are derived from experimental observation, there may be slight variation in values between different publications.

TABLE 10.2.1 Average bond enthalpies ($kJ\,mol^{-1}$) for single bonds at 25°C and 1 atm pressure

	H	C	N	O	F	S	Cl	Br	I
H	436								
C	414	346							
N	391	286	158						
O	463	358	214	144					
F	567	492	278	191	159				
S	364	289			327	266			
Cl	431	324	192	206	255	271	242		
Br	366	285		201	249	218	219	193	
I	298	228		201	280		211	178	151

TABLE 10.2.2 Average bond enthalpies ($kJ\,mol^{-1}$) for multiple bonds at 25°C and 1 atm pressure

C=C	614
C≡C	839
C=N	615
C≡N	890
C=O	804
N=N	470
N≡N	945
O=O	498

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Enthalpy changes associated with a chemical reaction can be understood in terms of the energy associated with making and breaking the chemical bonds during the reaction.

Consider the formation of hydrogen chloride:

$$H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$$

In this reaction, the covalent bonds in hydrogen (H–H) and chlorine (Cl–Cl) are broken and two new covalent bonds (H–Cl, H–Cl) are formed.

Using data from Table 10.2.1, the enthalpy change of this reaction can be calculated. Note that bond breaking requires energy; the process is endothermic, so the sign attached to the bond enthalpy value is positive. Conversely, bond formation is an exothermic process, so the sign attached to the bond enthalpy will be negative.

		Average bond enthalpy ($kJ\,mol^{-1}$)
bonds broken	1 × H–H	+436
	1 × Cl–Cl	+242
bonds formed	2 × H–Cl	2 × –431
enthalpy change		–184

Therefore, the thermochemical equation for this reaction can be written as:

$H_2(g) + Cl_2(g) \rightarrow 2HCl(g) \qquad \Delta H = -184\,kJ\,mol^{-1}$

The enthalpy change for a reaction is the overall difference in energy between the amount of energy absorbed to break bonds in the reactants and the amount of energy released when bonds are formed in making the products. This is given the following formula: $\Delta H = \Sigma$(bonds broken) – Σ(bonds formed)

Worked example 10.2.2

CALCULATING THE ENTHALPY CHANGE OF A REACTION USING AVERAGE BOND ENTHALPIES

Use data from Tables 10.2.1 and 10.2.2 on page 227 to determine if the reaction below is exothermic or endothermic and calculate the enthalpy change:

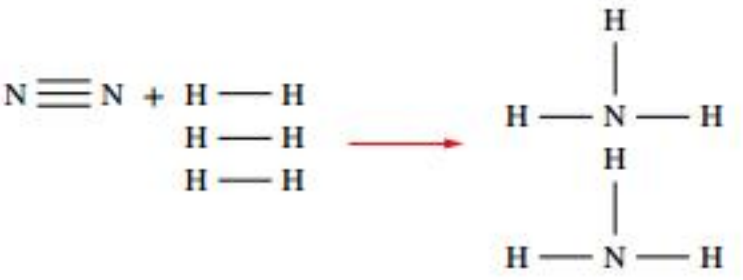
$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

Thinking

Draw molecules and identify the number and type of bonds broken and made.

Working

bonds broken	bonds formed
1 × N≡N	6 × N–H
3 × H–H	



Thinking

Use Tables 10.2.1 and 10.2.2 and record average bond enthalpy for each bond. Remember breaking bonds is endothermic, so average enthalpies will be +ve, while forming bonds is exothermic so average enthalpies will be –ve.

Working

		Average bond enthalpy ($kJ\,mol^{-1}$)
bonds broken	1 × N≡N	+945
	3 × H–H	3 × +436
bonds formed	6 × N–H	6 × –391

Thinking

Sum the values for bonds broken and bonds formed. Pay special attention to the signs of the bond enthalpy for each bond.

Working

		Average bond enthalpy ($kJ\,mol^{-1}$)
bonds broken	1 × N≡N	+945
	3 × H–H	+1308
bonds formed	6 × N–H	–2346
enthalpy change		–93

Thinking

Write ΔH, including the sign, and state the answer.

Working

$\Delta H = -93\,kJ\,mol^{-1}$

The reaction will be exothermic.

➤ Try yourself 10.2.2

CALCULATING THE ENTHALPY CHANGE OF A REACTION USING AVERAGE BOND ENTHALPIES

Use data from Tables 10.2.1 and 10.2.2 to determine if the reaction below is exothermic or endothermic and estimate the enthalpy change:

$$H_2(g) + F_2(g) \rightarrow 2HF(g)$$

Limitations in ΔH calculations

Using average bond enthalpies to calculate the enthalpy change of a reaction (ΔH) results in a value that is often quite different to the value determined experimentally. Remember that the average bond enthalpy is the amount of energy required to break one mole of bonds in the gaseous state under standard conditions, averaged for the same bond in different molecules. Since these are *average* bond enthalpies, the calculated ΔH is only an approximate value.

The limitations of using average bond energies such as those in Tables 10.2.1 and 10.2.2 on page 227 to calculate ΔH include the following:

- individual bond enthalpy values vary a little in different molecules because of the different chemical environments. For example, a C–H bond in one molecule will have a slightly different energy to the C–H bond in another molecule due to the effect of other electron groups (covalent bonds) around the C atom.
- bond enthalpy values are usually measured at 25°C, so if a reaction is at a different temperature the bond enthalpies will be slightly different.
- average bond enthalpies refer to the bonds in *gaseous* substances only, so the enthalpy changes caused by breaking intermolecular bonds in substances that are in a non-gaseous state are not accounted for.

Enthalpies of fuels

The transition to more sustainable fuels has to consider the effects on combustion of molecular structure and average bond enthalpies. The high energy content of diesel makes it an excellent fuel for transportation and equipment designed to do heavy work. For many years, petrodiesel, a fossil fuel, has been the primary source of fuel for diesel engines. Biodiesel, a fuel derived from plant material or animal fat, is now an alternative fuel to petrodiesel. These two fuels contain different molecules: Figure 10.2.7 shows the structural formula of an alkane, which is a typical component of petrodiesel, and the structural formula of a typical biodiesel molecule, a long-chain ester. The change over from petrodiesel to biodiesel is complicated by the fact that biodiesel, due to its structure and bond enthalpies, has a slightly lower ΔH. The reason for this is that all carbon atoms in petrodiesel will form high-energy C=O bonds during the combustion process shown below. However, two of the carbon atoms in biodiesel are already bonded to O atoms and so will not produce the energy associated with these two C=O bonds.

$$\text{fuel} + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g) + \text{energy}$$

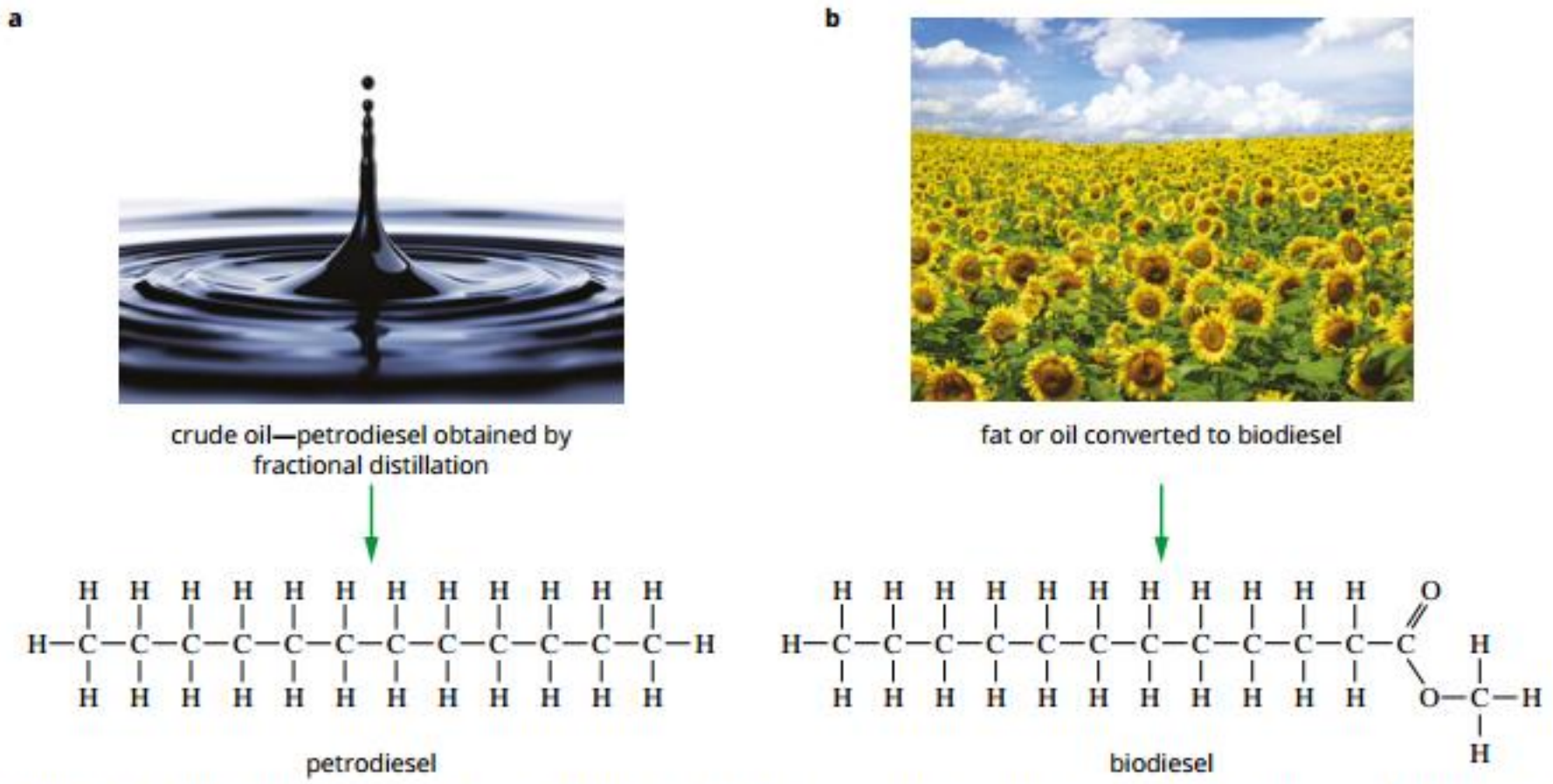


FIGURE 10.2.7 (a) Petrodiesel is generally composed of about 75% alkanes ranging from $C_{10}H_{22}$ to $C_{15}H_{32}$. (b) A typical biodiesel molecule is an ester molecule with a long carbon chain.

10.2 Review

SUMMARY

- The law of conservation of energy states that during any chemical or physical process, energy is neither created nor destroyed.
- In an exothermic reaction, energy will be released from the system into the surroundings because the total chemical energy of the products is less than the total energy of the reactants.
- In an endothermic reaction, energy will be absorbed from the surroundings because the total chemical energy of the products is greater than the total energy of the reactants.
- Enthalpy (H) is the chemical energy of a substance.
- Enthalpy change is given the symbol ΔH and is calculated using the equation $\Delta H = H_p - H_r$.
- Enthalpy level diagrams are used to represent the energy changes in a reaction.
- A thermochemical equation shows enthalpy change by writing the ΔH value to the right of the chemical equation. The ΔH value has the units $kJ\,mol^{-1}$.
- Breaking chemical bonds is an endothermic process, and making chemical bonds is an exothermic process.
- The energy required to break the bonds in the reactants is the activation energy.
- Bond enthalpy is the energy needed to break one mole of bonds of gaseous molecules under standard conditions (25°C, 1 atm pressure).
- Using average bond enthalpies in calculations gives an approximate enthalpy change because the values are averaged for different molecules and assume standard conditions and gaseous molecules.

KEY QUESTIONS

Describe

1 State the law of conservation of energy.

2 Define enthalpy.

3 What is the difference between a balanced chemical equation and a thermochemical equation?

Apply

4 Explain the term 'endothermic' in relation to the total amount of chemical energy of the reactants and products.

5 Explain why both exothermic and endothermic reactions require activation energy to proceed.

6 Explain why average bond enthalpies only give an approximation of the enthalpy change of a reaction.

7 When methane (CH_4) combusts, it reacts with oxygen to form carbon dioxide and water. The heat of combustion of methane is $-890\,kJ\,mol^{-1}$. Represent this reaction with a thermochemical equation.

8 Draw an enthalpy level diagram for the reaction described in Question **7**.

Analyse

9 Identify the following processes as exothermic or endothermic.

- **a** a reaction with a negative enthalpy change
- **b** burning methane
- **c** condensing steam
- **d** evaporating alcohol

10 Ammonium chloride, NH_4Cl, is readily soluble in water. The reaction with water is endothermic and can be represented by the equation:

$$NH_4Cl(s) \rightarrow NH_4^+(aq) + Cl^-(aq)$$

5.0 g of NH_4Cl is added to water and stirred until it dissolves.

- **a** Which bonds need to be broken for this reaction to occur?
- **b** Will this reaction absorb or release energy to the surroundings?
- **c** Will the temperature of the surroundings increase or decrease when this reaction occurs?

11 The thermochemical equation for photosynthesis can be represented as:

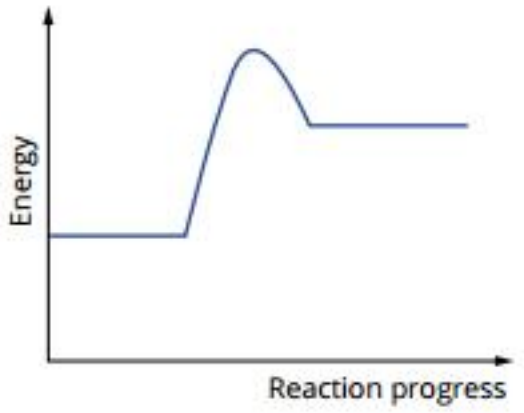
$$6CO_2(g) + 6H_2O(l) \xrightarrow[\text{chlorophyll}]{\text{light}} C_6H_{12}O_6(aq) + 6O_2(g)$$

$\Delta H = +2802.5\,kJ\,mol^{-1}$

- **a** Is this reaction endothermic or exothermic?
- **b** Consider a new reaction that reversed and halved the above reaction. It is written below. Calculate the energy change of the new reaction.

$$\frac{1}{2}C_6H_{12}O_6(aq) + 3O_2(g) \rightarrow 3CO_2(g) + 3H_2O(l)$$

12 The enthalpy level diagram below shows the energy changes during a reaction.



- **a** Is the reaction exothermic or endothermic?
- **b** Describe the relative enthalpies of the reactants and products.
- **c** Compare the size of the activation energy with ΔH.

13 Methane (CH_4) and methanol (CH_3OH) will both burn in air, according to the equations:

$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$

$\Delta H = -890\,kJ\,mol^{-1}$

$2CH_3OH(l) + 3O_2(g) \rightarrow 2CO_2(g)$ and $4H_2O(l)$

$\Delta H = -1452\,kJ\,mol^{-1}$

If 2 moles of methane and 2 moles of methanol are completely burned in separate experiments, which experiment will release the most energy?

14 Refer to the equations **A**, **B** or **C** to answer the questions below.

A $Br_2(g) \rightarrow Br_2(l)$

B $Br_2(g) \rightarrow 2Br(g)$

C $\frac{1}{2}Br_2(g) \rightarrow Br(g)$

- **a** Determine which equation describes the bond enthalpy of bromine.
- **b** Determine which equation describes the condensation of bromine.
- **c** Determine which change is exothermic.

15 In a steelworks, carbon monoxide present in the exhaust gases of the blast furnace can be used as a fuel elsewhere in the plant. It reacts according to the equation:

$CO(g) + \frac{1}{2}O_2(g) \rightarrow CO_2(g) \qquad \Delta H = -283\,kJ\,mol^{-1}$

- **a** Which has the greater total enthalpy: 1 mol of CO(g) and 0.5 mol of $O_2(g)$, or 1 mol of $CO_2(g)$?
- **b** Calculate the value of ΔH for the following equations:
  - **i** $2CO(g) + O_2(g) \rightarrow 2CO_2(g)$
  - **ii** $2CO_2(g) \rightarrow 2CO(g) + O_2(g)$

16 Identify the atoms involved in each bond and list the number of each of these bonds in the following molecule.

Name	Formula
hydrogen	H_2
water	H_2O
methane	CH_4
oxygen	O_2
ammonia	NH_3
carbon dioxide	CO_2

17 Use the average bond enthalpies in Tables 10.2.1 and 10.2.2 on page 227 to calculate the enthalpy change (ΔH) for each of the following reactions.

- **a** $2HF(g) \rightarrow H_2(g) + F_2(g)$
- **b** $2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$
- **c** $C(g) + 2H_2(g) \rightarrow CH_4(g)$

10.3 Measuring energy changes

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- explain Hess's law
- use Hess's law to calculate change in enthalpy
- understand the concept of specific heat capacity
- describe how calorimeters work
- use the equation $Q = mc\Delta T$ to calculate the enthalpy change measured using a calorimeter
- calculate the enthalpy change (ΔH) for a reaction given temperature changes, quantities of reactants and mass of water
- analyse data for heat of combustion, heat of neutralisation and reactions in aqueous solutions to determine heat, mass, specific heat capacity, temperature and enthalpy change

Have you ever wondered how the energy values on food nutrition labels, like those in Figure 10.3.1a, are calculated? The chemical potential energy of food, like that of all chemicals, is the energy stored in the bonds between the atoms. Chemical reactions can result in this energy being released and measured. In the case of food, the energy content can be measured by burning the food in a bomb calorimeter (Figure 10.3.1b).

FIGURE 10.3.1 (a) The energy values of a food are shown on its food label. (b) These values are measured by burning the food in a bomb calorimeter.

It is the quantitative understanding of how energy is absorbed and released on a molecular scale that is essential to understanding the heat flow that can be measured.

In this module, you will see how the energy changes of chemical reactions can be calculated and measured, both directly and indirectly.

HESS'S LAW

Sometimes it is difficult to measure the enthalpy change of a reaction. The reaction may occur too quickly or too slowly to measure, or it may be a brief intermediate step in a series of reactions. Fortunately, in 1840, the Swiss–Russian chemist Germain Henri Hess (1802–50) discovered that it is possible to determine the enthalpy of reaction indirectly. His discovery is known as **Hess's law**. Hess's law states that the amount of heat energy released or absorbed in a chemical reaction is constant, irrespective of the number of steps or the kind of steps by which the reaction is carried out, provided that the same reactants and products are involved.

According to Hess's law, if you add two or more thermochemical equations to give a final equation, then you can also add the enthalpy of reaction of these individual steps to give the final enthalpy of reaction.

The energy cycle in Figure 10.3.2 shows the consequence of Hess's law in that no matter the pathway of a chemical reaction, the difference in energy between two substances is independent of the route taken for the conversion. That is, $\Delta H_1 = \Delta H_2 + \Delta H_3$.

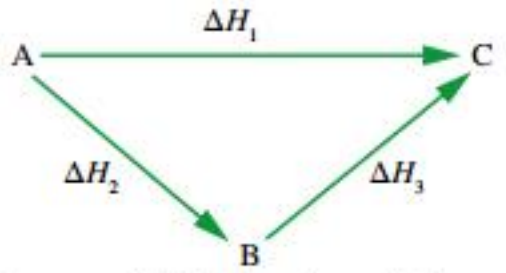


FIGURE 10.3.2 The difference in energy (ΔH) between two substances in a chemical reaction is independent of how they are converted. The diagram shows that the difference in energy between A and C (ΔH_1) is the same as the sum of the differences between A and B (ΔH_2), and B and C (ΔH_3).

Figure 10.3.3 shows a stepped energy diagram for the formation of carbon dioxide directly from carbon mixed with oxygen or the formation of carbon dioxide via carbon monoxide. It shows that whichever reaction pathway is taken to form carbon dioxide the amount of energy involved is the same.

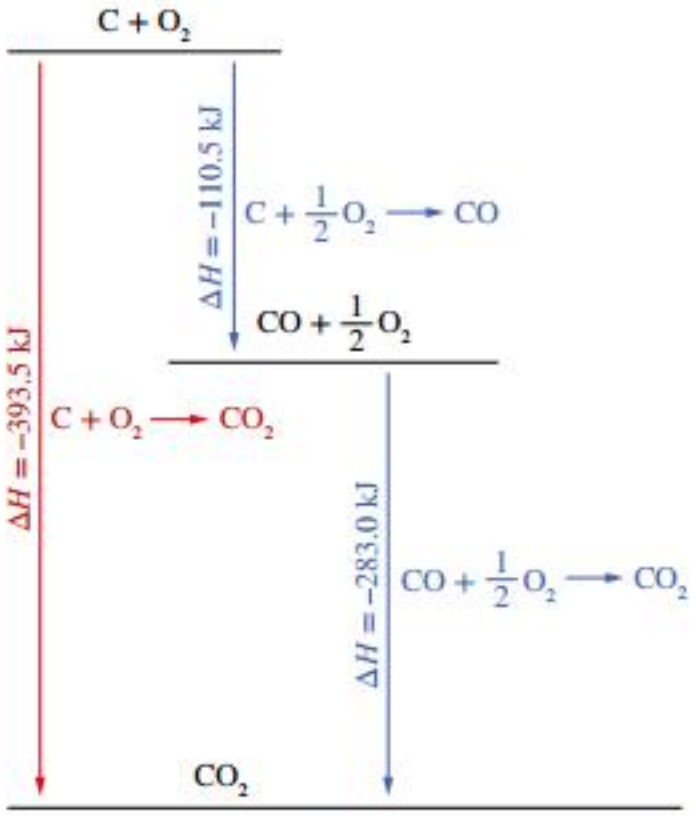


FIGURE 10.3.3 A stepped energy diagram for the formation of carbon dioxide from carbon and oxygen via carbon monoxide.

$$C(s) + \frac{1}{2}O_2(g) \rightarrow CO(g) \qquad \Delta H = -110.5\,kJ\,mol^{-1}$$

$$CO(g) + \frac{1}{2}O_2(g) \rightarrow CO_2(g) \qquad \Delta H = -283.0\,kJ\,mol^{-1}$$

$$C(s) + O_2(g) \rightarrow CO_2(g) \qquad \Delta H = -110.5 + (-283.0) = -393.5\,kJ\,mol^{-1}$$

This example demonstrates Hess's law as a restatement of the law of conservation of energy. The importance of Hess's law is that it allows the calculation of enthalpies that cannot be measured directly in the laboratory. Such calculations are based on three key properties of chemical reactions.

1 Chemical reactions are reversible if the appropriate conditions are available.
2 Energy is always involved in a chemical reaction. The products of an exothermic reaction contain less energy than the starting reactants: ΔH for an exothermic reaction is negative. Conversely, ΔH for the reverse endothermic reaction is positive.

For example, the combustion of carbon to form carbon dioxide can be reversed:

$C(s) + O_2(g) \rightarrow CO_2(g)$ $\quad \Delta H = -393.5\,kJ\,mol^{-1}$

$CO_2(g) \rightarrow C(s) + O_2(g)$ $\quad \Delta H = +393.5\,kJ\,mol^{-1}$

3 Equations for chemical reactions can be added and subtracted in the manner of ordinary algebraic equations such that complex chemical equations can be reduced to a series of simpler equations of formation with known enthalpies of reaction.

Worked example 10.3.1

USING HESS'S LAW TO CALCULATE THE ENTHALPY CHANGE OF A REACTION

Calculate the enthalpy change for the reaction:

$$S(s) + O_2(g) \rightarrow SO_2(g)$$

Use the following information.

$S(s) + \frac{3}{2}O_2(g) \rightarrow SO_3(g)$ $\quad \Delta H = -395\,kJ\,mol^{-1}$ (1)

$SO_2(g) + \frac{1}{2}O_2(g) \rightarrow SO_3(g)$ $\quad \Delta H = -98\,kJ\,mol^{-1}$ (2)

Thinking	Working
In this problem, you must find a path from S(s) to $SO_2(g)$. As the standard enthalpy change cannot be measured directly, an alternative route will enable you to determine the enthalpy change between S(s) and $SO_3(g)$. Reaction 1 gives you the correct starting point.	$S(s) + \frac{3}{2}O_2(g) \rightarrow SO_3(g)$ $\quad \Delta H = -395\,kJ\,mol^{-1}$
Reverse reaction 2 to give the correct final product, $SO_2(g)$. Remember to change the enthalpy sign.	$SO_3(g) \rightarrow SO_2(g) + \frac{1}{2}O_2(g)$ $\quad \Delta H = +98\,kJ\,mol^{-1}$
Combine the equations.	$S(s) + \frac{3}{2}O_2(g) + SO_3(g) \rightarrow SO_{3(g)} + SO_2(g) + \frac{1}{2}O_2(g)$ $\Delta H = -395 + 98\,kJ\,mol^{-1}$
Simplify.	$S(s) + \frac{3}{2}O_2(g) + SO_3(g) \rightarrow SO_{3(g)} + SO_2(g) + \frac{1}{2}O_2(g)$ $\Delta H = -297\,kJ\,mol^{-1}$
State the answer.	$S(s) + O_2(g) \rightarrow SO_2(g)$ $\quad \Delta H = -297\,kJ\,mol^{-1}$

➤ Try yourself 10.3.1

USING HESS'S LAW TO CALCULATE THE ENTHALPY CHANGE OF A REACTION

Calculate the enthalpy change for the reaction:

$$C(graphite) + \frac{1}{2}O_2(g) \rightarrow CO(g)$$

Use the following information.

$C(graphite) + O_2(g) \rightarrow CO_2(g)$ $\quad \Delta H = -394\,kJ\,mol^{-1}$ (1)

$CO(g) + \frac{1}{2}O_2(g) \rightarrow CO_2(g)$ $\quad \Delta H = -283\,kJ\,mol^{-1}$ (2)

CALORIMETRY

The enthalpy change in a chemical reaction can be measured experimentally using a technique called **calorimetry**. Calorimetry is the experimental method of measuring the heat energy released or absorbed by a chemical reaction or physical process, such as by the combustion of a fuel or the reaction between an acid and a base.

In the simplest form of calorimetry, the heat energy released by a chemical reaction can be transferred to water in a container. The quantity of energy transferred can be calculated from the increase in temperature of the water in the **calorimeter**.

The heat energy transferred to the mass of water can be calculated by measuring the:

- initial temperature of the water
- highest temperature of the water
- mass of water.

The relationship used to calculate the energy that has been transferred to the water is:

$$Q = m \times c \times \Delta T$$

where Q is the energy that is transferred to the water (in J), m is the mass of the water (in g), c is the specific heat capacity of the water ($4.18\,J\,g^{-1}\,°C^{-1}$), and ΔT is the change in temperature of the water (in °C or K):

$$\Delta T = T_{final} - T_{initial}$$

The **specific heat capacity** of a substance is a measure of the amount of energy (usually in joules) needed to increase the temperature of a specific quantity of that substance (usually 1 gram) by 1°C. It reflects the types of bonds holding the molecules, ions or atoms together in the substance.

Specific heat capacity is given the symbol c and is usually expressed in joules per gram per degrees Celsius, i.e. $J\,g^{-1}\,°C^{-1}$. It can also be expressed in joules per grams per kelvin, i.e. $J\,g^{-1}K^{-1}$ (an increase of 1°C is the same as an increase of 1 K).

The specific heat capacities of some common substances are listed in Table 10.3.1. You can see that the value for water is relatively high, which is a consequence of the hydrogen bonding between its molecules. You will also note that the metals, copper and lead, have much lower specific heat capacity because of their high conductivity.

TABLE 10.3.1 The specific heat capacity of some common substances

Substance	Specific heat capacity ($J\,g^{-1}\,°C^{-1}$)
water	4.18
glycerine	2.43
ethanol	2.46
sand	0.48
copper	0.39
lead	0.16

A calorimeter is an instrument designed to measure the energy changes in a reaction. Calorimetry is the experimental method of measuring heat energy released or absorbed by a chemical process.

The energy required to increase a known mass of substance by a particular temperature is given by the formula $Q = m \times c \times \Delta T$

where

Q = amount of energy in Joules (J)

m = mass in grams (g)

c = specific heat capacity ($J\,g^{-1}\,°C^{-1}$)

ΔT = temperature change (°C)

SKILLBUILDER 10.3.1

Using density to convert volume to mass

In Chemistry, glassware such as measuring cylinders, pipettes and burettes are used to measure volumes of liquids. Some calculations require the mass of a liquid such as water, so the density formula is needed to convert the measured volume to a mass.

The density of a substance is a measure of the mass that is contained in a certain volume of that substance. It is calculated using the formula $d = \frac{m}{V}$ where d is the density of the substance, m is the mass and V is the volume. Typical units are $g\,mL^{-1}$. Density can be measured for all substances and provided in a data table.

Converting volume to mass

Calculate the mass, in grams, of 30.2 mL of ethanol at 25°C given that the density of ethanol is $0.785\,g\,mL^{-1}$ at 25°C.

Step 1: State the given information and identify the quantity required. Check that the volume unit matches the unit in the density.

d(ethanol) = $0.785\,g\,mL^{-1}$

V(ethanol) = 30.2 mL

m(ethanol) = ?

Step 2: Recall the density formula and rearrange it.

$d = \frac{m}{V}$ so $m = d \times V$

Step 3: Substitute known values to calculate mass.

m(ethanol) = $d \times V$
= 0.785×30.2
= 23.7 g (to 3 significant figures)

Worked example 10.3.2

CALCULATING THE HEAT ENERGY REQUIRED TO HEAT A VOLUME OF WATER

Calculate the heat energy, in kJ, needed to increase the temperature of 255 mL of water by 18.0°C.	
Thinking	**Working**
Given that the density of water is $1.00\,g\,mL^{-1}$, convert the volume of water, in mL, to mass of water, in g.	$d = \frac{m}{V}$ So, $m = d \times V$ m(water) = $d \times V$ = 1.00×255 = 255 g
Recall that the specific heat capacity, c, of water can be found in Table 10.3.1 on page 235.	The specific heat capacity of water is $4.18\,J\,g^{-1}\,°C^{-1}$.
To calculate the quantity of heat energy in Joules, use the formula: $q = mc\Delta T$	$Q = 255 \times 4.18 \times 18.0$ = 1.92×10^4 J
Express the quantity of heat energy in kJ. Remember that to convert from J to kJ, you divide by 1000 (10^3).	$Q = \frac{1.92 \times 10^4}{1000}$ = 19.2 kJ

➤ Try yourself 10.3.2

CALCULATING THE HEAT ENERGY REQUIRED TO HEAT A VOLUME OF WATER

Calculate the heat energy, in kJ, needed to increase the temperature of 375 mL of water by 45.0°C.

Aqueous solutions

Energy changes that occur in reactions involving solutions can be measured with a **solution calorimeter**. A solution calorimeter may be as simple as a polystyrene foam coffee cup with a lid, as shown in Figure 10.3.4.

The insulation provided by the polystyrene foam prevents the transfer of heat to or from the surroundings of the calorimeter. The reaction is carried out in the calorimeter with an accurately known volume of water. The initial and final temperatures are measured and recorded, as are the amounts of reactants used.

If the temperature of the water in the calorimeter increases, the reaction occurring in the calorimeter is an exothermic reaction. The reaction has released heat energy, the water in the calorimeter has absorbed that energy and the temperature of the water has increased.

Similarly, if the temperature of the water in the calorimeter decreases, the reaction occurring in the calorimeter has absorbed energy from the water. In this case, the reaction is an endothermic reaction.

A coffee cup calorimeter has some limitations. The polystyrene container absorbs some heat, so the temperature change is lower than it would otherwise be and the calculated value for the heat released or absorbed by the reaction is lower than it should be.

Solution calorimetry is used in the laboratory to determine the enthalpy changes that occur when acids react with bases and solids dissolve in water. The construction of a laboratory solution calorimeter is shown in Figure 10.3.5. The stirrer is used to ensure the temperature of the water is uniform. The electric heater is used to determine the **calibration factor** of the calorimeter. For more accurate measurements of the heat change in a reaction, you have to first determine how much energy is required to change the temperature of the water by 1°C for the particular calorimeter in use. This is known as the calibration factor of the calorimeter.

Heat of neutralisation

The enthalpy change that occurs when an acid reacts with a base is called the heat of neutralisation.

The acid–base reaction between hydrochloric acid and sodium hydroxide is represented by the following thermochemical equation:

$$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l) \quad \Delta H = -56.2\,kJ\,mol^{-1}$$

This equation tells you that when 1 mol of HCl reacts with 1 mol of NaOH to produce 1 mol of H_2O, 56.2 kJ of heat energy is released. A solution calorimeter such as the one shown in Figure 10.3.5 can be used to measure the heat of neutralisation.

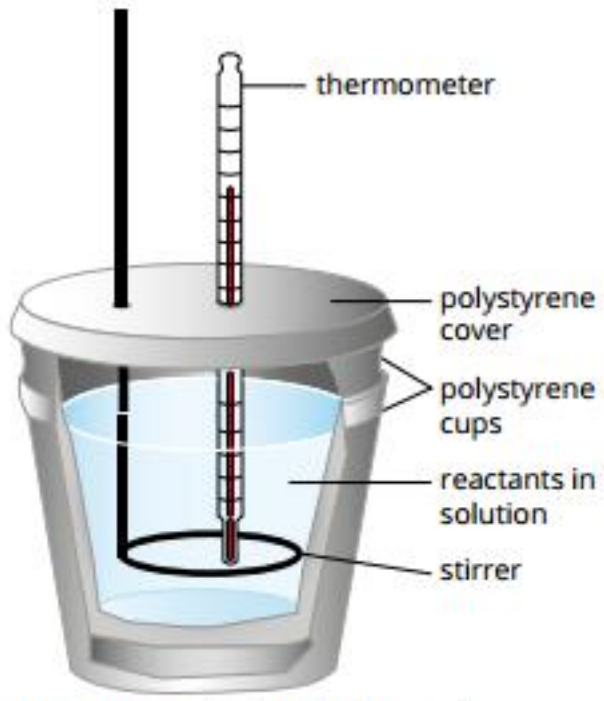


FIGURE 10.3.4 A simple 'coffee-cup' calorimeter.

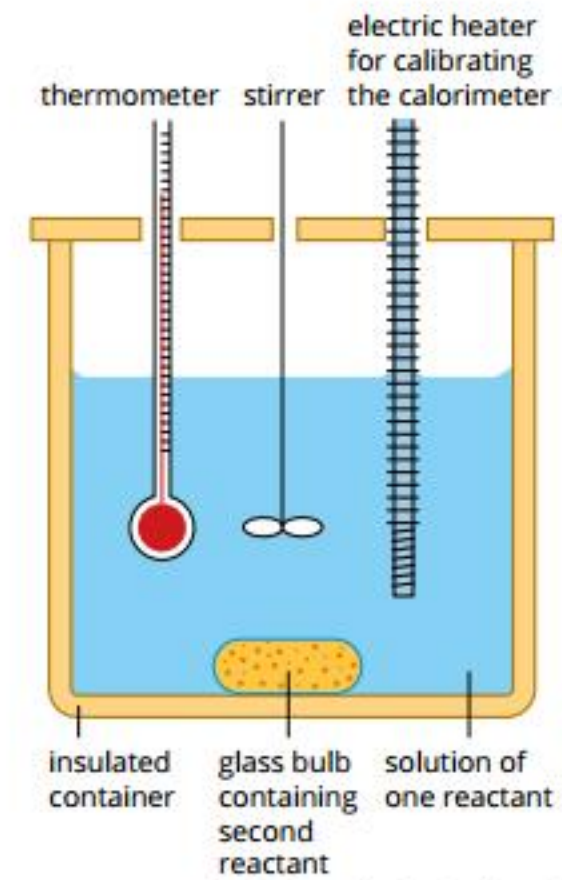


FIGURE 10.3.5 A solution calorimeter; breaking the glass bulb starts the reaction.

Worked example 10.3.3

CALCULATING HEAT OF NEUTRALISATION USING A SOLUTION CALORIMETER

A 25.0 mL sample of water containing 0.025 mol HCl at 25.0°C is added to another 25.0 mL sample of water containing 0.025 mol NaOH at 25.0°C in a 'coffee cup' calorimeter. A reaction occurs. The highest temperature recorded is 32.0°C. Calculate the heat of neutralisation, ΔH, in kJ mol^{-1}.

Assume the density of each solution is the same as water (1.00 g mL^{-1}) and the combined volume of the final solution is equal to the sum of the volumes of the reacting solutions.

Thinking	Working
The question is asking you to find the enthalpy change (ΔH). The first step is to list the information provided by the question.	$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O$ $T_i = 25.0°C$ $T_f = 32.0°C$ Volume = 25.0 + 25.0 = 50.0 mL $c = 4.18\,J\,g^{-1}\,°C^{-1}$ (Data from Table 10.3.1 on page 235)
Use the density formula $d = \frac{m}{V}$ to convert the volume to mass of water (m).	$d = \frac{m}{V}$ Rearrange the density formula to find m: $m = d \times V$ $= 1.00 \times 50.0$ $= 50.0\,g$
Use the formula $Q = m \times c \times \Delta T$ to calculate the energy transferred to the water. This is the heat gained by the water, but it is also the heat lost by the reacting HCl and NaOH, therefore change the sign to negative.	$\Delta T = T_f - T_i$ $= 32.0°C - 25.0°C$ $= 7.0°C$ $Q = m \times c \times \Delta T$ $= 50.0 \times 4.18 \times 7.0$ $= -1463\,J$
Now you need to find the heat released *per mole*. To calculate the energy per mole of acid or base, divide the number of joules by the number of moles.	$n(HCl) = n(NaOH) = 0.025$ mol $\Delta H = \frac{Q}{n}$ $= \frac{-1463}{0.025}$ $= -58\,520\,J$ $= -59\,kJ$ (to 2 significant figures) The heat of neutralisation is $-59\,kJ\,mol^{-1}$.

➤ Try yourself 10.3.3

CALCULATING HEAT OF NEUTRALISATION USING A SOLUTION CALORIMETER

When 50.0 mL of water containing 0.055 mol HCl at 22.5°C is mixed with 50.0 mL of water containing 0.055 mol NaOH at 22.5°C in a calorimeter, the temperature of the solution increases to 26.1°C. Calculate the heat of neutralisation, ΔH, in kJ mol^{-1}.

Assume the density of each solution is the same as water (1.00 g mL^{-1}) and the combined volume of the final solution is equal to the sum of the volumes of the reacting solutions.

HEAT OF COMBUSTION

Combustion reactions are rapid reactions between a fuel and oxygen. They are exothermic reactions that often release a large amount of energy. The **heat of combustion** is defined as the enthalpy change that occurs when a specified amount (e.g. 1 g, 1 L, 1 mol) of the fuel burns completely in oxygen. It is usually measured at conditions of 298 K (25°C) and 100 kPa (1 bar), which means that the water produced should be shown in the liquid state. The heat of combustion can be given the symbol ΔH_c.

Many fuels, including wood, coal and kerosene, are mixtures of chemicals and do not have a specific chemical formula or molar mass. This means their heat of combustion cannot be expressed in kJ mol^{-1}. Therefore, it is measured only as kJ g^{-1}, kJ L^{-1} or MJ/tonne.

The heats of combustion for some common elements and compounds present in fuels are listed in Table 10.3.2. Heat energy is released during combustion, so ΔH_c always has a negative value.

TABLE 10.3.2 Heats of combustion for some common elements and compounds

Substance	Heat of combustion, ΔH_c (kJ mol^{-1})
methane	–890
ethane	–1560
propane	–2220
butane	–2886
octane	–5450
methanol	–726
ethanol	–1367
hydrogen	–286
carbon (graphite)	–394

The heat of combustion of a substance can be measured using a copper calorimeter as shown in Figure 10.3.6. In a copper calorimeter, the heat released by the burning fuel is absorbed by the water above. The temperature of this water will increase, which allows the heat of combustion to be calculated using the formula:

$$\Delta H_c = \frac{Q}{n} = \frac{-mc\Delta T}{n}$$

A minus sign is placed before the m according to the convention that combustion reactions are always exothermic and will have negative enthalpy values.

Only fuels that exist as pure substances can have their heat of combustion measured in kJ mol^{-1}.

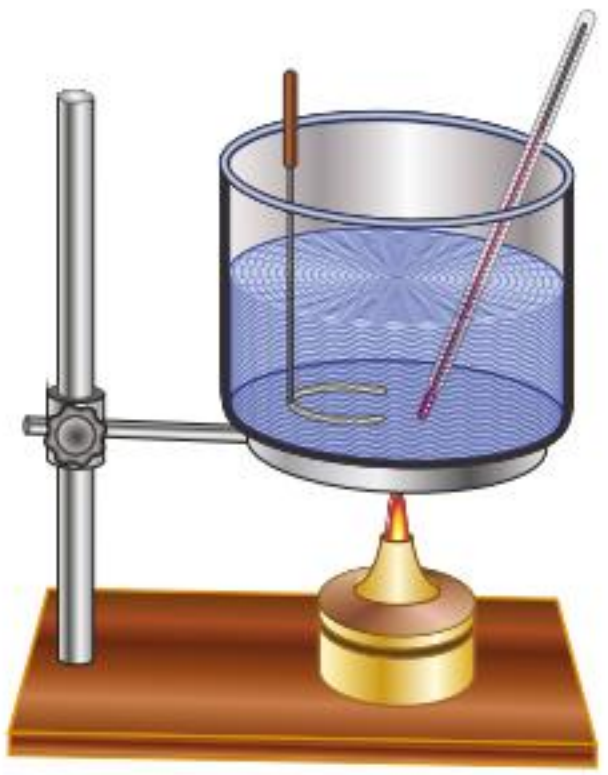


FIGURE 10.3.6 A copper calorimeter is used to measure the energy released by combustion reactions.

Worked example 10.3.4

CALCULATING THE HEAT ENERGY TRANSFERRED TO WATER FROM FUEL

A sample of fuel is used to heat 100 mL of water. Calculate the heat energy, in kilojoules, that has been transferred if the temperature of the water increases from 18.5°C to 44.0°C.

Thinking	Working
Change the volume of water in millilitres to mass of water in grams. Remember that the density of water is $1.00\,g\,mL^{-1}$.	1 mL of water has a mass of 1 g, so 100 mL of water has a mass of 100 g.
Calculate the change in temperature, ΔT, by subtracting the initial temperature from the final temperature: $\Delta T = T_f - T_i$	$\Delta T = T_f - T_i$ $= 44.0 - 18.5$ $= 25.5°C$
Calculate the heat energy transferred to the water, in joules, using the formula: $Q = m \times c \times \Delta T$	$Q = m \times c \times \Delta T$ $= 100 \times 4.18 \times 25.5$ $= 10659\,J$
Express the quantity of energy, in kJ, to the appropriate number of significant figures. Remember that to convert from joules to kilojoules, you divide by 10^3.	$Q = \frac{10659}{1000}$ $= 10.7\,kJ$ (3 significant figures)

➤ Try yourself 10.3.4

CALCULATING THE HEAT ENERGY TRANSFERRED TO WATER FROM FUEL

A sample of fuel is used to heat 200 mL of water. Calculate the heat energy, in kilojoules, that has been transferred if the temperature of the water increases from 15.5°C to 30.0°C.

Worked example 10.3.5

CALCULATING THE HEAT ENERGY PER GRAM TRANSFERRED TO WATER FROM A FUEL

A 0.850 g sample of fuel was burnt under a steel can containing 150 mL of water. After the flame went out, the mass of the fuel was 0.300 g and the temperature of the water had risen by 22.5°C. Calculate the energy content of the fuel in $kJ\,g^{-1}$.

Thinking	Working
Calculate the heat energy absorbed by the water in joules, using the formula: $Q = m \times c \times \Delta T$	$Q = m \times c \times \Delta T$ $= 150 \times 4.18 \times 22.5$ $= 14108\,J$
Express the quantity of energy in kJ. Remember that to convert from joules to kilojoules, you divide by 10^3.	$Q = \frac{14108}{1000}$ $= 14.108\,kJ$

Calculate the mass of the fuel that was burnt by subtracting the final mass from the initial mass: $\Delta m = m_i - m_f$	$\Delta m = m_i - m_f$ $= 0.850 - 0.300$ $= 0.550\,g$
Calculate the energy content of the fuel by dividing the energy transferred to the water by the change in mass during combustion: $\text{Energy content} = \frac{Q}{\Delta m}$	$\text{Energy content} = \frac{Q}{\Delta m}$ $= \frac{14.108}{0.550}$ $= 25.7\,kJg^{-1}$ (3 significant figures)

➤ Try yourself 10.3.5

CALCULATING THE HEAT ENERGY PER GRAM TRANSFERRED TO WATER FROM A FUEL

A 2.500 g corn chip was burnt under a steel can containing 200 mL of water. After the flame went out, the mass of the corn chip was 1.160 g and the temperature of the water had risen by 35.0°C. Calculate the energy content of the corn chip in kJg^{-1}.

Heat loss

When energy is transferred from burning a sample of fuel or food, across an open space, heat is lost to the surroundings such as the air. Similarly, if there is no lid on a container of water, heat will be lost from the surface of the water. This heat loss is illustrated in Figure 10.3.7.

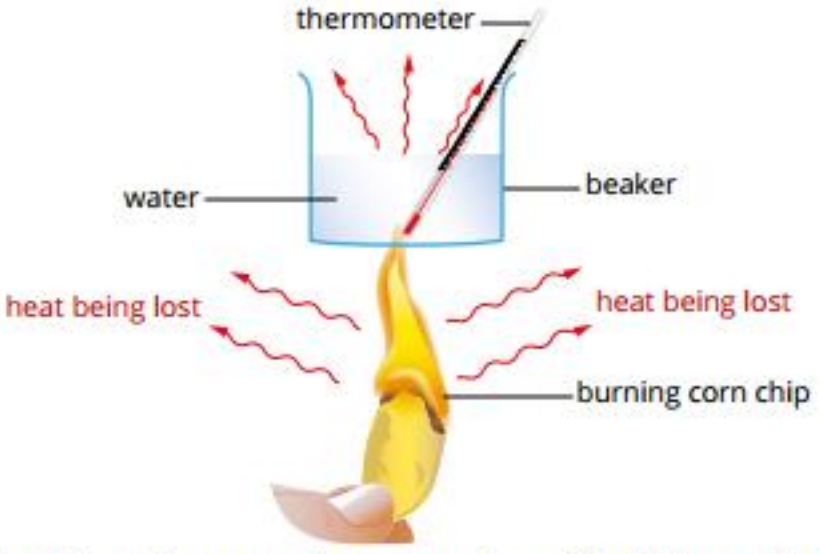


FIGURE 10.3.7 Heat is lost to the surroundings when a piece of food is burnt to heat some water.

When some heat energy from the burning fuel or food is transferred to the surrounding air, the temperature of the water does not increase as much as it would if all the energy was used to heat the water. A lower change in temperature, ΔT, of the water results in a lower energy value, Q.

There are several ways to reduce heat loss during the calorimetry experiment shown in Figure 10.3.7, including:

- putting a lid on the calorimeter
- insulating the beaker of water (with flameproof material)
- placing insulation around the burning food, although sufficient oxygen must reach the food for complete combustion to occur.

10.3 Review

SUMMARY

- According to Hess's law, if you add two or more thermochemical equations to give a final equation, then you can also add the enthalpy of reaction for each equation to give the overall enthalpy of reaction.
- Calculations involving Hess's law rely on three key properties of chemical reactions.
  1. Chemical reactions are reversible if the appropriate conditions are available.
  2. ΔH for an exothermic reaction is negative. ΔH for the reverse endothermic reaction is positive.
  3. Equations for chemical reactions can be added and subtracted in the manner of ordinary algebraic equations such that complex chemical equations can be reduced to a series of simpler equations of formation with known enthalpies of reaction.
- Calorimetry is the experimental method of measuring the heat energy released or absorbed in a chemical reaction or process.
- A calorimeter is an instrument designed to measure the energy changes in a reaction.
- The heat energy required to increase a given mass of water by a particular amount can be calculated using the equation:

$$Q = mc\Delta T$$

  where Q is heat energy (in J), m is mass of water to be heated (in g), c is the specific heat capacity of water ($4.18\,J\,g^{-1}\,°C^{-1}$) and ΔT is the temperature change (in °C).
- The enthalpy of reaction can be determined using a calorimeter: $\Delta H = \frac{Q}{n} = -\frac{mc\Delta T}{n}$.
- A solution calorimeter is an insulated container that holds a known volume of water and in which a reaction in solution can be carried out and the change in enthalpy measured.
- The heat of combustion is defined as the enthalpy change that occurs when a specified amount of the fuel burns completely in oxygen.
- Calculations of the enthalpy of reaction or the heat of combustion from experimental data can be very inaccurate due to heat loss to the surroundings during the experiment.

KEY QUESTIONS

Describe

1 Indicate if the following statement is true or false. 'According to Hess's law, if you add two or more thermochemical equations to give an equation, you cannot always add the enthalpy of each reaction to give the overall enthalpy of reaction.'

2 What is a calorimeter used for?

3 Describe a simple calorimeter that could be used to measure the enthalpy change of reactions between two solutions.

4 Define the term 'heat of combustion'.

Apply

5 Hess's law calculations rely on three fundamental properties of chemical reactions. Explain what they are.

6 Explain why water has a higher specific heat capacity than other substances.

Analyse

7 Refer to Table 10.3.1 on page 235 and state whether greater energy is required to raise the temperature of 20 g of copper or 20 g of lead by 1.0°C.

8 Calculate the enthalpy change, ΔH (in $kJ\,mol^{-1}$), for the following reaction:

$2NO(g) + O_2(g) \rightarrow 2NO_2(g)$

given the following enthalpy changes:

$N_2(g) + O_2(g) \rightarrow 2NO(g)$ $\quad \Delta H = +180.5\,kJ\,mol^{-1}$ (1)

$N_2(g) + 2O_2(g) \rightarrow 2NO_2(g)$ $\quad \Delta H = +66.4\,kJ\,mol^{-1}$ (2)

9 Calculate the enthalpy change, ΔH (in $kJ\,mol^{-1}$), for the following reaction:

$MnO_2(s) + C(s) \rightarrow Mn(s) + CO_2(g)$

given the following enthalpy changes:

$C(s) + O_2(g) \rightarrow CO_2(g)$ $\quad \Delta H = -390\,kJ\,mol^{-1}$ (1)

$Mn(s) + O_2(g) \rightarrow MnO_2(s)$ $\quad \Delta H = -520\,kJ\,mol^{-1}$ (2)

10 Calculate the mass, in grams, of 55 mL of ethanol at 25°C given that the density of methanol is $0.785\,g\,mL^{-1}$ at 25°C.

11 Calculate the energy required to increase the temperature of the following.

- **a** 100 mL of water by 15.2°C
- **b** 500 mL of water from 16.0°C to 28.0°C
- **c** 1.50 kg of water from 20.0°C to 30.0°C

12 When 2.35 kJ of heat energy is used to heat a mass of water in a beaker, the temperature changes by 6.1°C. Calculate the mass of water in the beaker.

13 When 100 mL of water containing 0.35 mol NaOH solution is added to 100 mL of water containing 0.35 mol HCl in a calorimeter, the temperature increases from 24.0°C to 49.5°C. Calculate the heat of neutralisation, ΔH, in kJ mol^{-1}.

Assume the density of each solution is the same as water (1.00 g mL^{-1}) and the combined volume of the final solution is equal to the sum of the volumes of the reacting solutions.

14 Determine the energy content, in kJ g^{-1}, of a wafer biscuit if combustion of 5.00 g of biscuit heats 500 mL of water by 38.3°C.

15 If the heat of combustion of a sample of coal is 20.7 kJ g^{-1}, what is the mass of coal that is burned when 62.7 kJ of energy is transferred to a container of water? Assume that all the energy from the burning coal is absorbed by the water.

Chapter review

10

KEY TERMS

activation energy
average bond enthalpy
boiling point
bond enthalpy
calibration factor
calorimeter
calorimetry
Celsius scale
change of state
chemical energy
combustion
condensation
deposition
endothermic
energy
enthalpy
enthalpy change
enthalpy level diagram
evaporation
exothermic
freezing
fuel
gas
gaseous
heat
heat content
heat of combustion
heat of neutralisation
heat of reaction
Hess's law
hydrocarbon
intermolecular bond
joule
Kelvin scale
kinetic theory
law of conservation of energy
liquid
melting
product
reactant
solid
solution calorimeter
specific heat capacity
state of matter
state symbols
sublimation
surroundings
system
temperature
thermochemical equation
thermochemistry
vaporisation
vapour

KEY QUESTIONS

Describe

1 Describe what is meant by the term 'system'.

2 Define the concept of temperature.

3 Define the concept of heat.

4 Identify whether each of the following statements related to activation energy is true or false.

a Activation energy is the energy required to break bonds in the reactants.

b Reactions that start immediately do not have an activation energy.

c Reactions that release energy overall do not need to absorb activation energy.

d The match used to light a fire is providing activation energy.

5 When butane is used as a fuel in some camp stoves, it reacts with oxygen. Compared with the total chemical energy of the combustion products, the total chemical energy of the reactants is:

A higher and the process is exothermic
B higher and the process is endothermic
C lower and the process is exothermic
D lower and the process is endothermic

6 Define specific heat capacity.

7 The equation $Q = m \times c \times \Delta T$ describes the relationship between heat energy and the temperature change of a substance being heated. It is used to determine how much energy has been absorbed by a material, such as a mass of water, when its temperature increases by a measured amount.
Which one of the following statements about this equation is correct?

A The specific heat capacity, *c*, depends on the material that is generating the heat energy.
B The mass, *m*, represents the mass of the material that is being heated.
C Q is measured in $kJ\,°C^{-1}$.
D ΔT refers to the change in temperature of the fuel generating the heat.

Apply

8 Which one of the following is correct about the energy profile diagrams of both endothermic and exothermic reactions?

A There is always less energy absorbed than released.
B The enthalpy of the products is always less than the energy of the reactants.
C Some energy is always absorbed to break bonds in the reactants.
D The ΔH value is the difference between the enthalpy of the reactants and the highest energy point reached on the energy profile.

9 Your fingers feel cold when you touch an ice cube. Explain the important thermochemical principle that this change illustrates.

10 Determine whether the following processes are exothermic or endothermic. Explain your answers.

a burning of wood
b melting of ice
c recharging of a car battery
d decomposition of plants in a compost heap

11 Water boils at 100°C. This means that it boils at:

A 0K
B 100K
C 273K
D 373K

12 The heat content of oils such as olive oil and canola oil can be determined by calorimetry. Suggest why the heat content of fuels such as oils are measured in $kJ\,g^{-1}$ and not $kJ\,mol^{-1}$.

Analyse

13 Explain why steam at 100°C has greater energy content than water at 100°C.

14 Convert the energy values to the units specified (to 3 significant figures).

a 2205J to kJ
b 0.152kJ to J
c 1890000J to MJ
d 0.0125MJ to kJ

15 Explain the difference between evaporation and boiling.

16 A particular reaction absorbs heat. This means that:

A the bonds made are stronger than the bonds broken
B the bonds broken were stronger than the bonds made
C ΔH is positive and heat is released
D ΔH is negative and heat is absorbed

17 Refer to the average bond enthalpies in Tables 10.2.1 and 10.2.2 on page 227 to answer the following questions:

a Do the average bond enthalpies refer to bond-breaking or bond-forming processes?
b Is bond-breaking an exothermic or an endothermic process?
c Is the bond enthalpy for a double bond simply twice the bond enthalpy of a single bond for the same atoms? Provide two specific examples to support your answer.
d Why are enthalpy changes (ΔH) calculated using the bond enthalpies in Tables 10.2.1 and 10.2.2 considered to be approximate values?

18 Use the heats of combustion in Table 10.3.2 on page 239 to write balanced thermochemical equations for the combustion in oxygen, $O_2(g)$, of each of the following fuels. The products are $CO_2(g)$ and $H_2O(l)$.

a propane, $C_3H_8(g)$
b ethane, $C_2H_6(g)$
c methanol, $CH_3OH(l)$

19 A kettle is filled with 855mL of water. Calculate the energy required to boil the water if the initial temperature of the water is 18.5°C. Assume that the water will boil at 100°C.

20 The combustion reaction of ethyne gas that occurs in a welding machine can be represented by the thermochemical equation:

$2C_2H_2(g) + 5O_2(g) \rightarrow 4CO_2(g) + 2H_2O(l)$
$\Delta H = -2619\,kJ\,mol^{-1}$

a Is this reaction endothermic or exothermic?
b Determine the new value of ΔH if the equation is written as follows:
$4C_2H_2(g) + 10O_2(g) \rightarrow 8CO_2(g) + 4H_2O(l)$

21 The combustion of butane gas in portable stoves can be represented by the thermochemical equation:

$2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(l)$
$\Delta H = -5772\,kJ\,mol^{-1}$

a How does the overall energy of the bonds in the reactants compare with the overall energy of the bonds in the products?
b Draw an enthalpy level diagram for the reaction, labelling ΔH and activation energy.

22 Calculate the enthalpy change for the following reaction using the average bond energies from Tables 10.2.1 and 10.2.2 on page 227:

$C(g) + O_2(g) \rightarrow CO_2(g)$

23 Explain why reversing a chemical reaction reverses the sign of ΔH.

24 Calculate the enthalpy change (ΔH) in $kJ\,mol^{-1}$ for the following reaction:

$2Al(s) + Fe_2O_3(s) \rightarrow 2Fe(s) + Al_2O_3(s)$

given the following enthalpy changes:

$2Al(s) + \frac{3}{2}O_2(g) \rightarrow Al_2O_3(s)$
$\Delta H = -1676.0\,kJ\,mol^{-1}$ (1)

$2Fe(s) + \frac{3}{2}O_2(g) \rightarrow Fe_2O_3(s)$
$\Delta H = -822.1\,kJ\,mol^{-1}$ (2)

25 Calculate the energy needed to heat the following.

a 100mL of water from 20.0°C to 80.0°C
b 2300g of water from 18.0°C to 100.0°C
c 300g of cooking oil from 18.0°C to 100.0°C ($C_{(\text{cooking oil})} = 2.2\,J\,g^{-1}\,°C^{-1}$).

26 The density of ethanol, C_2H_5OH, is $0.785\,g\,mL^{-1}$ at 25°C and has a specific heat capacity of $2.46\,J\,g^{-1}\,°C^{-1}$.
- **a** Calculate the mass of ethanol that fills a 75 mL container.
- **b** If an equal amount of energy is used to heat 100 g of water and 100 g of ethanol, explain which liquid would have the higher increase in temperature.
- **c** Calculate the energy required to raise the temperature of 0.15 L of ethanol by 25°C.

27 Which one of the following is most likely to be the temperature change in 100.0 mL of water in a beaker with no insulation and no lid, when 2.10 kJ of energy is produced by burning a biscuit under the beaker?
- **A** 3.20°C
- **B** 5.02°C
- **C** 5.50°C
- **D** 6.30°C

28 An aluminium mass is heated and placed into a cup calorimeter containing 40.0 mL of water at 17.0°C. The water reaches a temperature of 20.0°C. Calculate the amount of energy (in J) released.

29 A 0.254 g piece of black coal was burnt and used to heat 300 mL of water. The temperature of the water rose from 18.25°C to 24.92°C. Calculate the heat of combustion, in $kJ\,g^{-1}$, of the coal. Assume all of the heat released during combustion was used to heat the water.

Interpret

30 A 2.5 g sample of a hydrocarbon mixture was completely burnt in a calorimeter containing 750 mL of water. The initial temperature of the water was 18°C. The temperature of the water once all the fuel had been used was 46°C.
- **a** Is this an endothermic or an exothermic reaction?
- **b** Will ΔH will be positive or negative for this reaction?
- **c** Determine the amount of energy (in kJ) that was used to heat the water, assuming all the energy from the combustion reaction was transferred to the water.

31 A 500 mL volume of water in a beaker was heated using the energy released by the combustion of a 3.00 g piece of wood. The observed temperature rise was 22.9°C.
- **a** Determine the heat of combustion of wood in $kJ\,g^{-1}$ and in $MJ\,t^{-1}$.
- **b** Determine if the heat of combustion you calculated in part **a** would be higher or lower than the actual heat of combustion of the wood. Give reasons for your answer.

Data analysis

DATA SET 1

The information below applies to Questions 1–5.

A student set up the apparatus shown in Figure 1 to determine the heat of combustion of ethanol, CH_3CH_2OH.

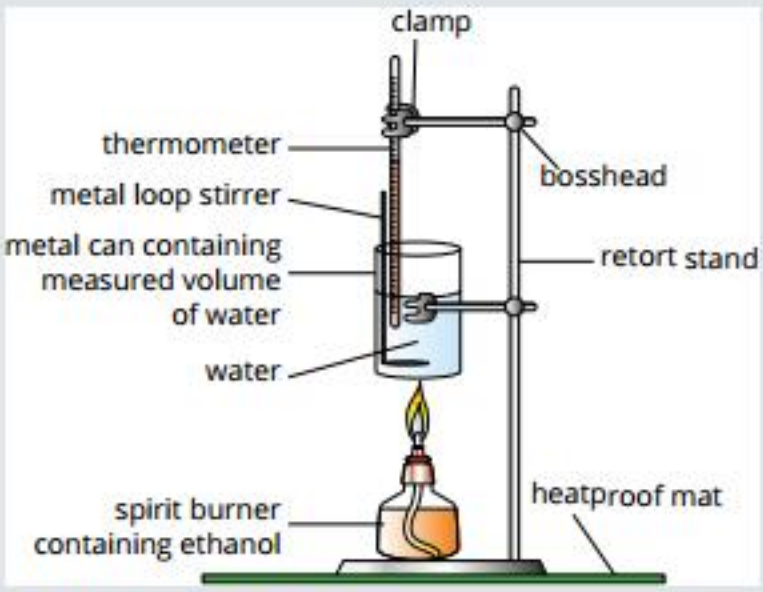


FIGURE 1 Apparatus for determining the heat of combustion of ethanol.

The experimental data collected by the student is shown in Table 1.

TABLE 1 Logbook data for combustion of ethanol

Initial mass of burner and ethanol	221.413 g
Final mass of burner and ethanol	219.112 g
Volume of water heated	250.0 mL
Initial temperature of water	19.0°C
Final temperature of water	59.5°C

Data required to calculate the heat of combustion is provided in Table 2.

TABLE 2 Data book extract

Specific heat capacity of water	$4.18\,J\,g^{-1}\,°C^{-1}$
Density of water	$1.00\,g\,mL^{-1}$

Question 1 (3 marks)

Use the experimental data to calculate the heat of combustion (ΔH_c) of ethanol in $kJ\,g^{-1}$. Express your answer to an appropriate number of significant figures.

Question 2 (2 marks)

The value for the heat of combustion of ethanol in chemical databases is 29.6 $kJ\,g^{-1}$. Calculate the percentage of heat lost to the surroundings in this experiment.

Question 3 (2 marks)

Identify two sources of error in this experiment that would account for the percentage heat loss calculated in Question 2.

Question 4 (1 mark)

Describe how the experimental design could be improved to minimise one of the errors identified in Question 3.

Question 5 (2 marks)

Evaluate the validity of the result in terms of the experimental design and the results obtained.

REVIEW QUESTIONS

Chemical fundamentals—structure, properties and reactions

Topic 1: Properties and structure of atoms

Multiple-choice questions

1 Compare the electronegativity and the first ionisation energy of caesium, Cs, and barium, Ba.

A Cs is less electronegative and has a lower first ionisation energy.
B Cs is more electronegative and has a higher first ionisation energy.
C Cs is less electronegative and has a higher first ionisation energy.
D Cs is more electronegative and has a lower first ionisation energy.

2 Select the case in which the radius of the first-named species is smaller than the radius of the second-named species.

A chloride ion (Cl^-); chlorine atom (Cl)
B iron(II) ion (Fe^{2+}); iron(III) ion (Fe^{3+})
C magnesium atom (Mg); magnesium ion (Mg^{2+})
D potassium ion (K^+); potassium atom (K)

3 Determine the effective nuclear charge of an atom that has the electronic structure $1s^2 2s^2 2p^6 3s^2 3p^4$.

A 2
B 4
C 6
D 16

4 Consider the following oxides:

Al_2O_3, Cl_2O, Na_2O

Identify the sequence that correctly lists these oxides in order, from left to right, from basic to amphoteric to acidic.

A Al_2O_3, Cl_2O, Na_2O
B Cl_2O, Na_2O, Al_2O_3
C Na_2O, Al_2O_3, Cl_2O
D Cl_2O, Al_2O_3, Na_2O

5 Consider the following electrostatic forces:

I attraction between oppositely charged particles
II repulsion between positively charged particles
III repulsion between negatively charged particles

The electrostatic forces operating in an atom are:

A I only
B I and II
C I and III
D I, II and III

Use the following information for Questions 6 and 7.
The atomic number, mass number and electron configuration of four particles, W, X, Y and Z, are given below.

	Atomic number	Mass number	Electron configuration
W	17	37	$1s^2 2s^2 2p^6 3s^2 3p^6$
X	19	39	$1s^2 2s^2 2p^6 3s^2 3p^6$
Y	17	37	$1s^2 2s^2 2p^6 3s^2 3p^5$
Z	19	40	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$

6 Identify the correct statement.

A W is a noble gas.
B X is a positively charged ion.
C Y is in group 5 of the periodic table.
D Z is a negatively charged ion.

7 Identify the particles that are isotopes of the same element.

A W and X
B X and Z
C Y and Z
D W, X and Y

8 Consider two unknown elements, A and B. Element A is in group 4 of the periodic table. Element B is in group 16. Deduce the most likely formula for a compound between A and B.

A A_4B_{16}
B $A_{16}B_4$
C AB_4
D AB_2

9 The formula for hydrogen cyanide is HCN. Deduce the number of electrons shared between the carbon and nitrogen atom.

A 2
B 4
C 6
D 8

10 Select the pair of elements that will form an ionic compound.

A sulfur with oxygen
B copper with tin
C tin with chlorine
D carbon with chlorine

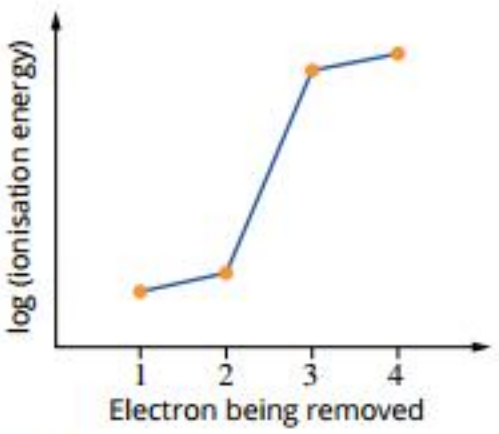
11 Bromine has two stable isotopes, ^{79}Br and ^{81}Br. It has a relative atomic mass of 79.90. The percentage of ^{81}Br in a sample of naturally occurring bromine is closest to:

A 30%
B 50%
C 60%
D 80%

12 Copper has two isotopes, ^{63}Cu and ^{65}Cu. It has a relative atomic mass of 63.55. Any one particular copper atom will:

A contain either 63 or 65 protons
B contain either 34 or 36 neutrons
C have a mass number of 63.55
D have an atomic number of 29 or 31

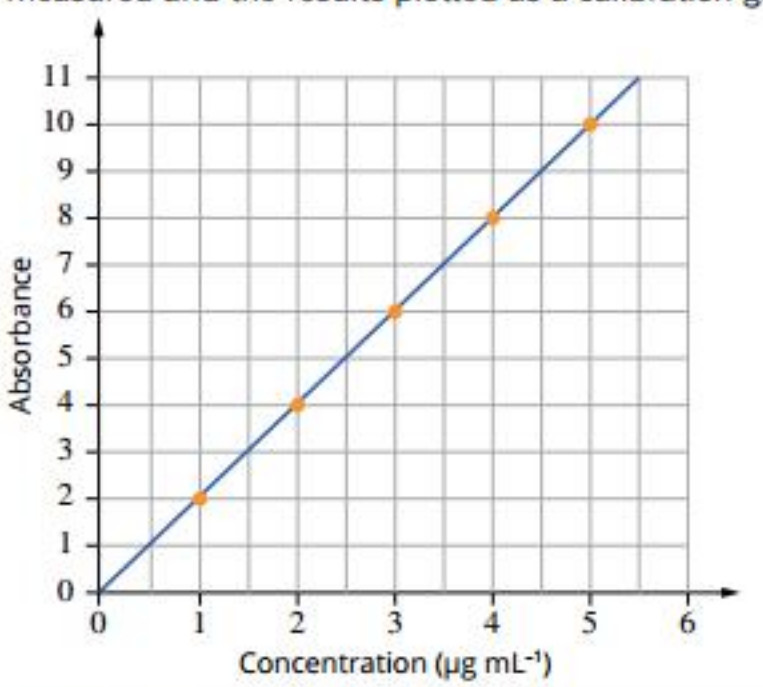
13 A plot of the first four ionisation energies of an element is shown below.



The element could be:

A oxygen
B aluminium
C sodium
D magnesium

14 Cadmium is a toxic heavy metal, which can cause kidney disease. The concentration of cadmium ions in river water was determined using atomic absorption spectrometry (AAS). The absorbance values of several solutions of known concentration of cadmium ions were measured and the results plotted as a calibration graph.



A sample of river water had an absorbance of 5.0. The cadmium ion concentration, in $\mu g\,mL^{-1}$, in the sample of water is:

A 2.0
B 2.5
C 5.0
D 10.0

15 When a salt was heated in the flame of a Bunsen burner, the flame colour changed to an intense yellow. Identify the salt.

A barium chloride
B calcium chloride
C potassium chloride
D sodium chloride

16 Zinc is an element. Determine which statement is true.

A Zinc has no isotopes.
B All zinc atoms are identical.
C Zinc atoms always contain the same number of protons.
D Zinc atoms contain equal numbers of protons and neutrons.

Short-answer questions

1 An isotope of rubidium, $^{85}_{37}Rb$, is ionised to yield the Rb^+ ion.

a How many electrons are present in the Rb^+ ion?
b Explain the meaning of the term 'isotope'.
c Write the symbol of another possible isotope of rubidium using nuclear symbol notation.

2 Consider an atom of chlorine.

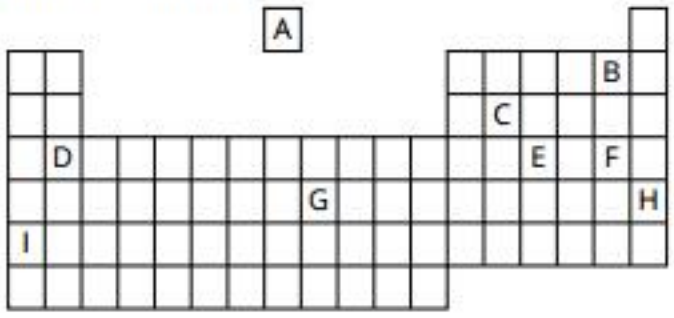
a What is its atomic number?
b Write the electron configuration of the atom.
c How many orbitals in *p* subshells are occupied by electrons?
d If there are 18 neutrons in the nucleus of the atom, write its nuclear symbol notation.
e What would be the charge of the ion if the atom gains one electron?

3 **a** With the aid of a periodic table, identify the correct chemical symbol for each of the following.

i The element that is in group 2 and period 4.
ii A noble gas with exactly three occupied electron shells.
iii An element from group 14 that is a non-metal.
iv An element that has exactly three occupied electron shells and is in the *s* block.
v The element in period 2 that has the largest atomic radius.
vi The element in group 15 that has the highest first ionisation energy.
vii The element in period 2 with the highest electronegativity.

b Describe the trend in chemical reactivity of elements going down group 1 of the periodic table and give a brief explanation for this trend.

4 Below is an outline of the periodic table, with a number of elements identified using letters that are not their normal symbols. Use these letters when answering the following questions.



a Select the element that has the highest electronegativity.

b Identify the elements that have an electron configuration ending in s^2p^5.

c Identify the element that does not usually react with other elements.

d Select the element that has an electron configuration of $1s^22s^22p^63s^23p^63d^{10}4s^24p^3$.

5 Complete the table below by placing a tick (√) in the box that correctly describes the trend in the property listed as you move down a group and across a period from left to right.

Property	Trend in property			
	down a group		across a period (from left to right)	
	increase	decrease	increase	decrease
atomic radius				
ionisation energy				
electronegativity				
metallic character				
non-metallic character				
ease of formation of positive ions				
ease of formation of negative ions				
acidic nature of oxides				

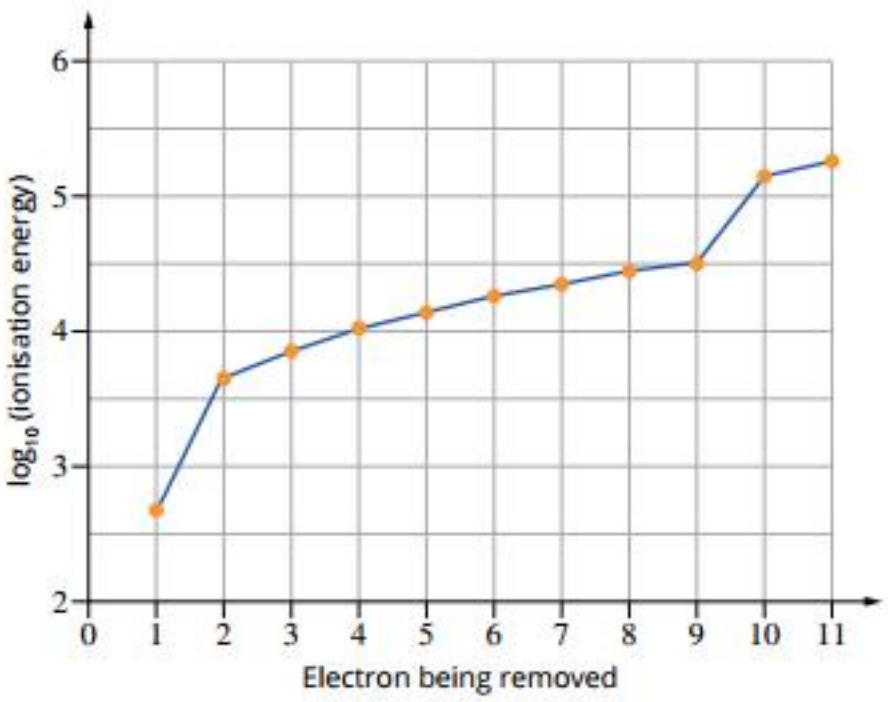
6 The ionic radii of some ions are provided in the following table.

Ion	Ionic radius (pm)	Number of protons	Electron configuration
N^{3-}	146		
O^{2-}	140		
F^-	133		
Na^+	102		
Mg^{2+}	72		
Al^{3+}	53		

a Complete the table by indicating the number of protons in the nucleus of each ion and the electron configuration of each ion.

b Suggest a reason why the ionic radii decrease down this set of ions.

7 The graph below shows the successive ionisation energies for sodium.



Use the information provided in this graph to explain how the energies for the successive ionisation of sodium are related to its electronic structure.

8 **a** Using an atom of sodium as an example, clearly explain the difference between an electron shell, a subshell and an orbital.

b What is the effect of the Pauli exclusion principle on electrons in orbitals?

c Consider the following electron configuration: $1s^22s^22p^63s^23p^63d^1$.

i Deduce if this electron configuration represents a ground state or excited atom.

ii Give a reason for your answer.

9 This question concerns two elements, identified as X and Y. Information about ions of these two elements is shown in the table below.

Element	Mass number	Atomic number	Number of neutrons	Number of electrons
X	24	12	i	10
Y	ii	15	16	iii

a Supply the following information to complete the table.
- **i** Determine how many neutrons are in an atom of X.
- **ii** Determine the mass number of an atom of Y.
- **iii** Determine how many electrons the Y^{3-} ion contains.
- **iv** Give the symbol for the ion formed by X.

b **i** Deduce the group in the periodic table to which element X belongs.
- **ii** Deduce the period in the periodic table to which element Y belongs.

c Explain why an atom of X has a larger radius than an atom of Y.

10 Using your knowledge of trends in the periodic table, explain why the element rubidium (Rb) has a lower first ionisation energy value than lithium and iodine.

11 Why is nitrogen unable to form all three types of chemical bonds: metallic, covalent and ionic?

12 Explain the relationship between the electronegativity difference and the acidic nature of an oxide, using the elements Li and F in your answer.

13 **a** Write the formula of each of these compounds.
- **i** potassium sulfate
- **ii** aluminium oxide
- **iii** sodium nitrate
- **iv** iron(III) sulfide

b Write the name of each of these compounds.
- **i** $Ca(NO_3)_2$
- **ii** $CuCO_3$
- **iii** $Mg(OH)_2$
- **iv** Cr_2O_3

c The formula of the ionic compound calcium phosphide is Ca_3P_2.
- **i** Write the formula for the phosphide ion.
- **ii** Provide the ground state electron configuration of the phosphide ion.

14 Discuss this statement in terms of ionic and covalent bonding, using potassium chloride and chlorine as examples: 'All chemical bonding is electrostatic in nature.'

15 Draw the Lewis structure and state the number of bonding pairs and non-bonding pairs of electrons for the following species.
- **a** O_2
- **b** NH_4^+
- **c** HF

16 Iridium has two naturally occurring isotopes. Their relative isotopic masses and percentages abundances are shown in the table below.

Isotope	Relative isotopic mass	Percentage abundance (%)
^{191}Ir	190.97	37.30
^{193}Ir	192.97	62.70

a Recall the name of the instrument that is commonly used to experimentally obtain the abundances and relative isotopic masses data.

b Using the information in the table, determine the relative atomic mass of iridium. Show your working and give your answer to the appropriate number of significant figures.

17 Lithium has two isotopes. Their relative isotopic masses are 6.02 and 7.02. The relative atomic mass of lithium is 6.94. Calculate the relative abundance of the lighter isotope.

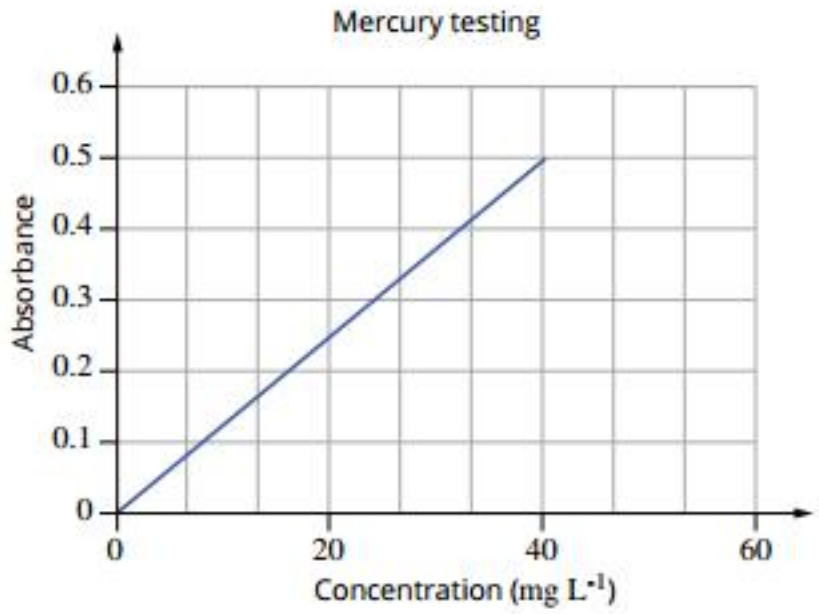
18 **a** Describe how Bohr used evidence from spectral analysis to propose his model of the atom.

b State the name given to the set of lines found in the visible region of the hydrogen emission spectrum. Describe the electron transitions that generate these lines.

c Describe one way in which the Schrödinger model of the atom differs from that of Bohr's model.

19 Deep-sea fish can build up high levels of mercury from contaminated water. A 3.0g sample of fish is ground up and mixed with water. The mixture is made up to 100mL with water. A sample of the solution is analysed by atomic absorption spectroscopy, giving an absorbance reading of 0.23.

Use the following calibration curve to determine the quantities below.



a percentage mass of mercury in the fish

b concentration in ppm of mercury in the fish.

20 Atomic absorption spectroscopy was used to determine the concentration of sodium ions in ground water.

The absorbance readings of a series of standard solutions are shown in the table below.

Concentration of sodium ($mg\,L^{-1}$)	Absorbance
2.0	0.14
4.0	0.28
6.0	0.42
8.0	0.56
10.0	0.70

a Identify what evidence there is in the data to indicate that the calibration graph is linear.

b Plot the calibration graph.

c Determine the concentration of sodium in a sample that had an absorbance of 0.38.

21 The atomic number of four elements, I, II, III and IV, and their atomic radii are provided in the following table. Refer to the information in this table when answering parts **a** and **b**.

Element	I	II	III	IV
Atomic number	11	19	20	35
Atomic radius	186	227	147	114

a Complete the following table by writing the electron configuration of these elements in the long and short form.

Element	Long form	Short form
I		
II		
III		
IV		

b Describe, using elements I, II, III and IV as examples, how the structure of the periodic table is determined by the atomic number and the properties of the elements. Identify the group and period to which each of the four elements belongs.

c Explain why the periodic table consists of four blocks and why the number of columns within each block differs.

22 Describe and explain the trends in atomic radii in the periodic table. Your answer should include the following points.

- Explain the meaning of the term 'effective nuclear charge' and outline how this may be calculated.
- Explain the role of effective nuclear charge in determining the radius of an atom.
- Identify and explain other factors that determine the radius of atoms.
- Illustrate your answer with appropriate examples using the elements in the table in Question **21**.

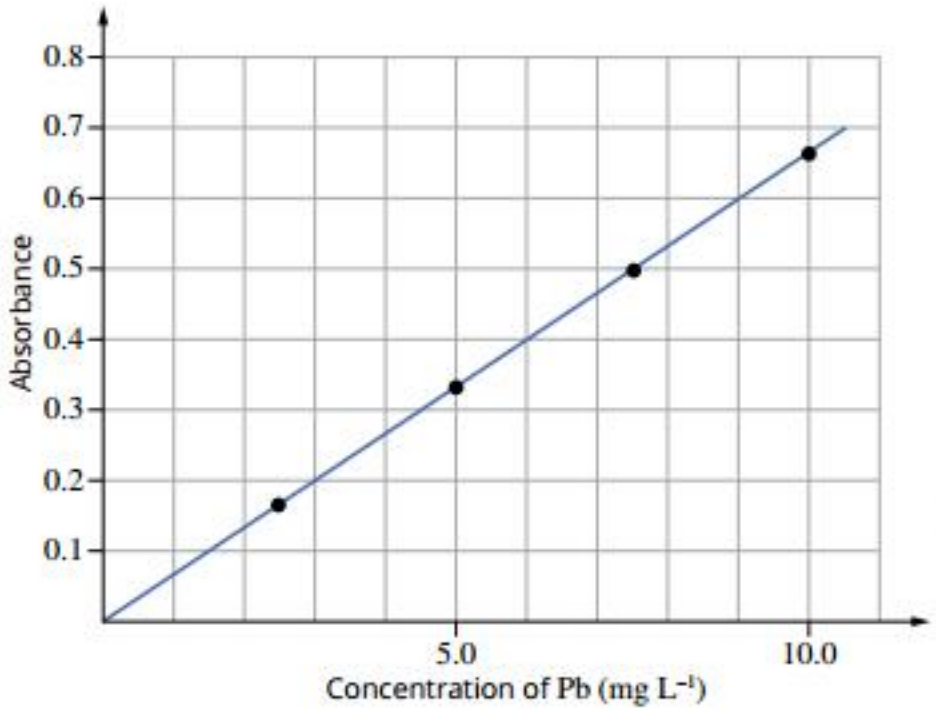
23 **a** Use orbital diagrams to illustrate the application of the Aufbau principle, Hund's rule and the Pauli exclusion principle in the determination of the electron configuration of sodium, carbon and iron.

b Identify two elements that have an electron configuration different from that predicted by the Aufbau principle. Provide the actual and predicted electron configurations for each element.

24 Mass spectrometry and atomic absorption spectrometry are two analytical techniques used by chemists. Compare these two techniques by:

- describing the information provided by each technique
- outlining the basic principles upon which each technique is based.

25 The lead level in a sample of contaminated soil was investigated using atomic absorption spectrometry. A 3.0g sample was dissolved in acid and then diluted to a total volume of 25.0mL. The absorbance of this solution, determined in a spectrometer set at an appropriate wavelength, was found to be 0.40. Several standard solutions of lead were tested under the same conditions and the calibration curve shown below was generated.



a Determine the mass of lead present in the 3.0g sample.

b Determine the concentration of lead in the soil as %(m/m).

c Explain why it was necessary to construct a calibration curve in this investigation.

26 Briefly discuss the difference between the emission and absorption spectrum of hydrogen. Describe, in terms of electron transitions, how each spectrum is generated.

27 A student set up an experiment to determine the flame colour of each of the compounds in the table below.

Compound	Flame colour
NaCl	yellow
$CaCl_2$	brick-red
KCl	lilac

The student then crushed a piece of chalk and recorded these observations in their log book:

Initially, the flame changed to a brownish-red colour when the sample of crushed chalk was inserted and then the flame changed back to the original blue colour observed.

a Determine which individual species (ion, atom or compound) they should conclude was present in the chalk.

b Briefly explain why some compounds change the colour of a flame.

28 The concentration of zinc in soil can be determined using an atomic absorption spectrometer. Standard solutions were prepared and their absorbance recorded in the table below. The soil sample gave an absorbance reading of 0.40.

Concentration of standard solution ($mg\,L^{-1}$)	Absorbance
0.00	0.00
1.00	0.16
2.00	0.32
3.00	0.48
4.00	0.64

a Construct a calibration curve.

b Determine the concentration of zinc in the soil sample.

29 When a sample of palladium is placed in a mass spectrometer, several peaks are recorded as the relative isotopic masses and their corresponding percentage abundances. These are recorded in the table below.

Relative isotopic mass	Percentage abundance (%)
101.9049	0.9600
103.9036	10.97
104.9046	22.23
105.9032	27.33
107.9039	26.71
109.9044	11.80

Calculate the relative atomic mass of palladium and express your answer to 4 significant figures.

Topic 2: Properties and structure of materials

Multiple-choice questions

1 The atoms of an element have the electron configuration:

$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^2 5s^2$

The solid state structure of the element is best described as

A a covalent network lattice

B an ionic lattice

C a molecular lattice

D a metallic lattice

2 One or more of the following bonds are a consequence of electrostatic attractions. Which one(s)?

A hydrogen bonds

B ionic bonds

C covalent bonds

D metallic bonds

E all of the above

3 Select the statement about solids, liquids and gases that is incorrect.
- **A** Liquids and gases are both fluids and they can be poured.
- **B** Solids and liquids have a definite volume but gases have a variable volume.
- **C** Solids are incompressible but liquids and gases are highly compressible.
- **D** Solids have a definite shape, but liquids and gases have variable shapes.

4 Select the correct statement about the boiling points of pure water and salt water.
- **A** The boiling points of pure water and salt water are the same.
- **B** The boiling point of pure water is less than the boiling point of salt water.
- **C** The boiling points of pure water and salt water depend upon the volume of the liquids.
- **D** The boiling point of pure water remains constant, while the boiling point of salt water decreases as more salt is added.

5 You have been provided with two solutions. Solution A contains 1 g of NaCl dissolved in 50 mL of water. Solution B contains 5 g of NaCl dissolved in 100 mL of water. Select the statement that correctly describes the difference between the properties of solutions A and B.
- **A** Solution A has a higher boiling point than solution B.
- **B** Solution A has a lower electrical conductivity than solution B.
- **C** Solution A has a higher density than solution B.
- **D** Solution A has a lower freezing point than solution B.

6 Identify the statement that does NOT apply to ionic bonding.
- **A** When molten, ionic compounds are conductors of electricity.
- **B** An ionic lattice contains both cations and anions in fixed positions.
- **C** Ionic bonding involves the sharing of electrons between two different atoms.
- **D** Compounds held together by ionic bonding generally have high melting temperatures.

7 It would be possible to tell whether the particles in a compound were held together by ionic or covalent bonds by measuring which characteristic of the compound?
- **A** melting temperature
- **B** hardness and brittleness
- **C** electrical conductivity in the solid state
- **D** electrical conductivity in the liquid (molten) state

8 Identify the member of the alkane family.
- **A** C_2H_4
- **B** C_3H_8
- **C** C_6H_6
- **D** C_8H_{16}

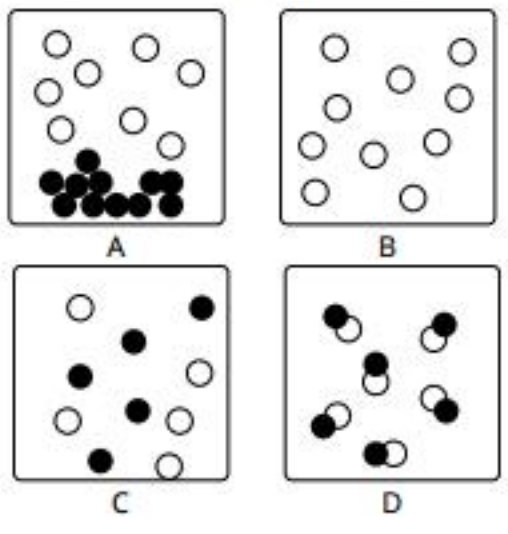
9 Predict which one of the following ionic compounds will have the highest melting point.
- **A** MgO
- **B** $MgCl_2$
- **C** Na_2O
- **D** NaCl

10 A white substance that is used in sunscreen has a melting point of 1975°C. It does not conduct electricity when solid and it does not dissolve in water. Which of the following would be an experimental observation that could be made to confirm without doubt that this substance is ionic?
- **A** The solid white substance is very hard.
- **B** The white substance conducts electricity when it is molten.
- **C** The solid white substance is brittle and shatters when hit with a hammer.
- **D** The solid white substance conducts heat well.

11 Which of the following lists of ions and their names is completely correct?
- **A** nitride (NO_3^-), ammonium (NH_4^+), copper (Cu_2^+)
- **B** oxide (O^{2-}), nitrate (NO_3^{2-}), silver (Ag^{2+})
- **C** sulfide (SO^{2-}), nitrite (NO_3^-), nickel (Ni^{2+})
- **D** iron(II) (Fe^{2+}), sulfate (SO_4^{2-}), nitride (N^{3-})

Short-answer questions

1 Two different elements are represented in the following diagram as black and white circles.



Match each of the following with the appropriate diagram, A, B, C or D.
- **a** a pure substance
- **b** an element
- **c** a compound
- **d** a heterogeneous mixture
- **e** a homogeneous mixture

2 **a** Classify each of the following substances by placing a tick in the appropriate place in the table below.

Substance	Element	Compound	Homogeneous mixture	Heterogeneous mixture
salt water				
silver				
concrete				
sugar				
oil and water				
air				

b Deduce which of the substances listed in the table are pure substances.

3 Ionic compounds have a variety of uses in everyday life.

a Give the formula and a use of one ionic compound.

b Use the ionic bonding model to explain the following properties of ionic compounds.

i Solid ionic compounds cannot conduct electricity.

ii Ionic compounds are generally brittle.

iii Ionic compounds have high melting temperatures.

4 Magnesium is a commonly used structural metal.

a The radius of a magnesium atom is 160 pm (1 pm = 10^{-12} m). Convert the radius of the magnesium atom to nanometres (1 nm = 10^{-9} m).

b i Describe the model commonly used to describe the structure of metals such as magnesium and the nature of the bonding between its particles. You may include a labelled diagram in your answer.

ii Use the metallic bonding model to explain why magnesium is a good conductor of electricity.

iii The metallic bonding model is useful to explain many of the properties of metals. However, like most models, it has some limitations. Give one example of a limitation of the metallic bonding model.

c Magnesium is most commonly used as an alloy for structural purposes. Define an alloy. Give one example of how alloying affects the properties of a metal.

5 Which one or more of the following substances contain(s) metallic bonding?

lithium, diamond, steel, neon, salt, calcium oxide, sulfur, calcium

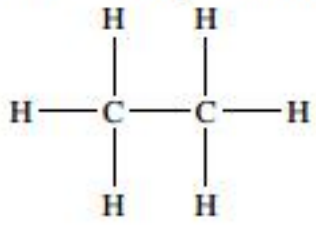
6 Explain the difference between the structure of diamond and that of a fullerene.

7 Explain the following observations in terms of structure and bonding.

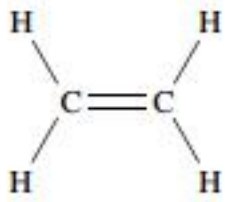
a Nickel chloride only conducts electricity when molten or in aqueous solution, not when solid.

b Diamond is widely used as an abrasive on the ends of drill bits.

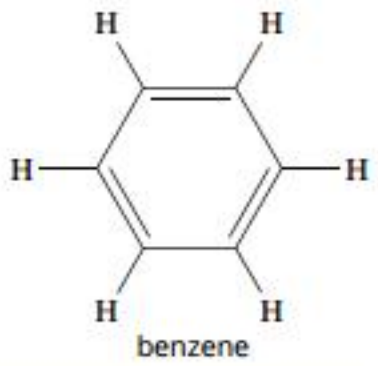
8 Complete the table below by matching the names of the three hydrocarbons with their bond energies, bond length and reactivity with bromine.



ethane



ethene



benzene

Hydrocarbon	C–C bond energy ($kJ\,mol^{-1}$)	Bond length (pm)	Reaction with Br_2
	356	154	no reaction
	636	134	reaction
	518	140	no reaction

9 The properties of some substances are described below.

a Substance W is hard, brittle and does not conduct electricity, and it sublimes at approximately 3500°C.

b Substance X melts at 645°C and does not conduct electricity in the solid state, but conducts electricity when molten.

c Substance Y melts at 842°C, and conducts in both the solid and liquid states.

d Substance Z is a diatomic gas at room temperature and does not conduct electricity in either the solid or liquid states.

Identify and describe the type of bonding in each substance and explain the properties listed in terms of the type of bonding.

10 Consider the following molecules: oxygen (O_2) and nitrogen (N_2).

a Draw the Lewis structure of each molecule.

b Unlike nitrogen atoms, oxygen atoms do not form triple bonds in molecules. Explain why with reference to the number of valence electrons in these two atoms.

11 Duralumin is a light but strong metal used in the manufacture of aircraft parts and racing bikes. It is an alloy of aluminium, containing around 4% copper and 1% magnesium and manganese.

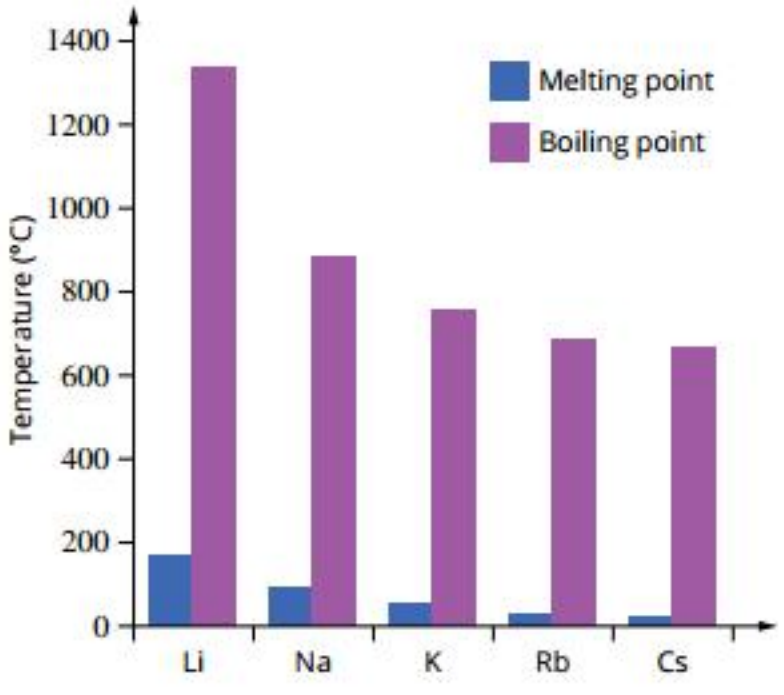
- **a** Describe the structure and bonding in Duralumin.
- **b** Explain why Duralumin is:
  - **i** malleable
  - **ii** able to conduct electricity
- **c** Duralumin is harder than aluminium. Account for the difference in terms of structure and bonding.

12 Diamond and graphite are allotropes of carbon. Although they are similar in some respects, they are very different in their structure and uses.

- **a** Give a brief definition of the term 'allotrope'.
- **b** Describe the similarity in the bonding of these two materials.
- **c** Compare the structures of diamond and graphite.
- **d** Graphite is an excellent conductor of electricity, while diamond is unable to conduct electricity. In terms of the structure of their lattices, explain this difference.
- **e** Graphite is used as lead in pencils. With reference to the bonding in the lattice, explain why graphite can be used in this way.
- **f** Describe the structure of graphene.

13 Strontium is a metallic element that has the following properties. It is a soft silvery-grey solid. It has a melting point of 776.9°C and a boiling point of 1382°C. It has a density of 2630 kg m^{-3}. It reacts vigorously on contact with water and tarnishes in air. Classify the listed properties of strontium as physical or chemical.

14 Examine the graph below that shows the melting and boiling points of the group 1 elements.

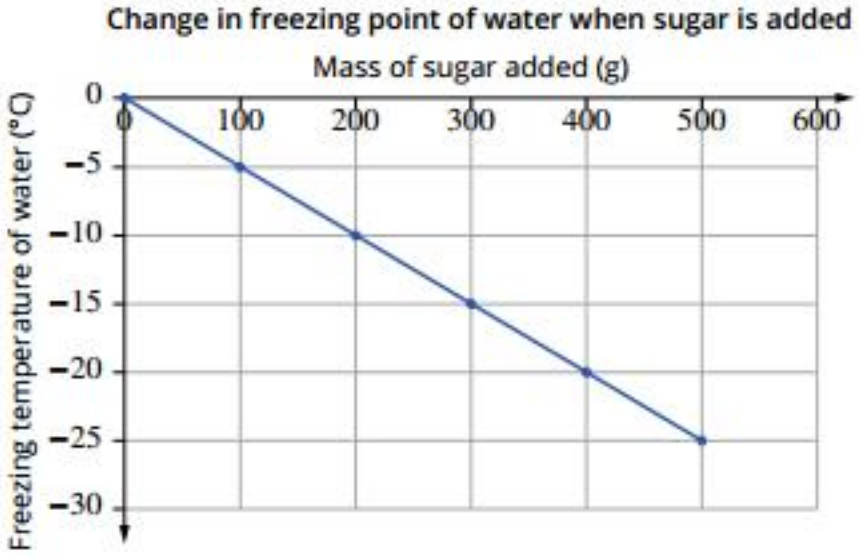


- **a** Describe the trend that is shown in the graph.
- **b** If you were to add francium to the graph, predict its melting point and boiling point.

Potassium and sodium can be made into an alloy that is used as a catalyst in some organic reactions. The alloy has a lower melting point than either of the elements.

- **c** Would an alloy of potassium and sodium be classified as a pure substance or a mixture. Explain your answer.
- **d** You have a sample of a grey solid that could be either sodium or an alloy of potassium and sodium. Propose a method to test the identity of the grey solid.

15 When sugar is added to water, it lowers the freezing point of the water; this is especially useful when making ice cream or desserts. A student investigated the change in the freezing temperature of water for different masses of sugar. In each trial, the student added the sugar to 1000 g of distilled water. The results of the investigation are shown in the graph below.



- **a** Describe the trend in the data.
- **b** The student wishes to make ice cream and needs the water to freeze between −6°C and −10°C. What is the minimum amount of sugar the student should add to achieve this?

Topic 3: Chemical reactions—reactants, products and energy change

Multiple-choice questions

1 Identify the set of coefficients (w, x, y, z) that would balance the following equation:

$$w C_2H_5OH(l) + x O_2(g) \rightarrow y CO_2(g) + z H_2O(l)$$

- **A** 1, 3, 2, 3
- **B** 2, 7, 4, 6
- **C** 2, 6, 4, 5
- **D** 1, 6, 2, 3

2 The reaction of sodium sulfite with hydrochloric acid may be represented by the equation:

$Na_2SO_3(s) + 2HCl(aq) \rightarrow 2NaCl(aq) + H_2O(l) + SO_2(g)$

On the basis of the information in the equation, identify the correct statement.

A When 1 mol of Na_2SO_3 is treated with acid, 1 mol of SO_2 will always be produced.

B Na_2SO_3 and H^+ must always be present in the mole ratio of 1:2 for a reaction to take place.

C The ratio by mass of Na_2SO_3 to H^+ in a reaction mixture containing the correct stoichiometric proportions is 1:2.

D 0.4 mol of H_2O will be produced when 0.8 mol of H^+ reacts completely with excess Na_2SO_3.

3 Identify the statement that best defines the empirical formula of a molecular compound.

A actual number and type of each element present

B simplest whole number mole ratio of each ion present

C simplest whole number mole ratio of each element present

D simplest whole number mass ratio of each element present

4 Determine which one of the following quantities contains the same number of ions as there are in 1 mol of NaOH.

A 1 mol of Na_2S

B 0.5 mol of K_3PO_4

C 1 mol of $MgCl_2$

D 1.5 mol of MgO

5 A particular brand of plant fertiliser contains 58.5% urea ($CO(NH_2)_2$) as the only nitrogen-containing compound. Determine the mass of nitrogen, in g, in 125 g of this fertiliser.

A 34.1

B 40.0

C 50.0

D 73.1

6 Determine the mass, in g, of calcium chloride that contains 6.02×10^{23} chloride ions.

A 35.5

B 55.6

C 75.6

D 111

7 A 54 g sample of hydrogen cyanide, HCN, combines with 80 g of oxygen to produce 18 g of water, 28 g of nitrogen and carbon dioxide, but nothing else. Calculate the mass of carbon dioxide produced.

A 44 g

B 88 g

C 134 g

D 286 g

8 In an experiment to determine the empirical formula of a chloride of a metal *X*, a student reduces 0.277 g of the chloride of *X* to the metal *X* itself. They obtain 0.207 g of *X*.

(relative atomic masses: *X* = 207; Cl = 35)

From these results, the formula of the compound is shown to be:

A XCl

B XCl_2

C XCl_3

D XCl_4

9 The combustion of 1 mol of ethanol, CH_3CH_2OH, in excess oxygen generates 1364 kJ of heat energy. Select the correct thermochemical equation for the reaction.

A $CH_3CH_2OH + 2O_2 \rightarrow 2CO_2 + 3H_2O$
$\Delta H = +1364\ kJ\ mol^{-1}$

B $CH_3CH_2OH(l) + 2O_2(g) \rightarrow 2CO(g) + 3H_2O(l)$
$\Delta H = -1364\ kJ\ mol^{-1}$

C $CH_3CH_2OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l)$
$\Delta H = -1364\ kJ\ mol^{-1}$

D $CH_3CH_2OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l)$
$\Delta H = +1364\ kJ\ mol^{-1}$

10 The thermochemical equation for the combustion of methanol in excess oxygen is:

$CH_3OH(l) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$
$\Delta H = -726\ kJ\ mol^{-1}$

Calculate the mass of methanol that must be consumed to produce 1.00 MJ of heat energy.

A 0.726 g

B 22.9 g

C 23.2 g

D 44.1 g

11 Which of the following statements are true for an exothermic reaction?

I The system absorbs heat.

II The enthalpy change is negative.

III The reactants are more stable than the products.

A II only

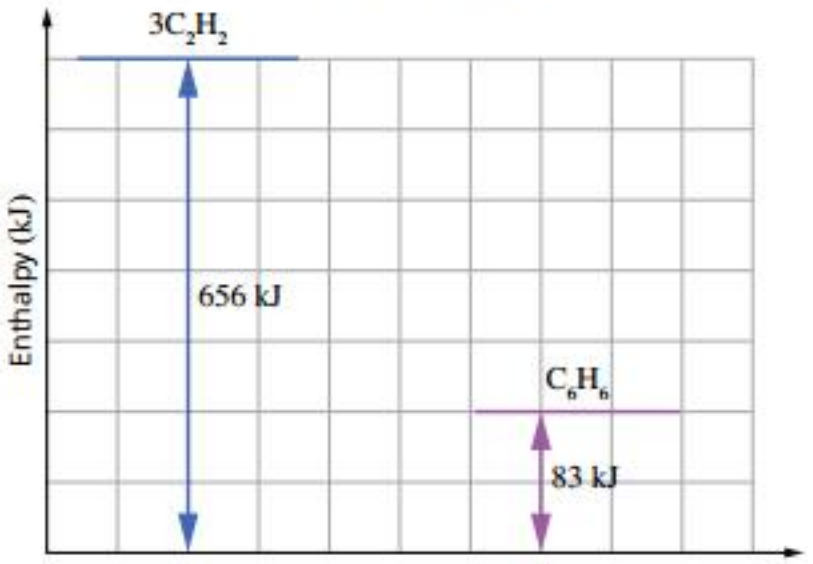
B I and II

C II and III

D I, II and III

12 Use the information in the diagram to determine ΔH for the reaction below:

$$3C_2H_2(g) \rightarrow C_6H_6(g)$$



A +739 kJ
B +573 kJ
C −573 kJ
D −656 kJ

13 For the reaction $2NH_3(g) \rightarrow N_2(g) + 3H_2(g)$; $\Delta H = +92\,kJ\,mol^{-1}$, select the correct statement.

A When 4 mol of ammonia decomposes, 92 kJ of heat will be evolved.
B When 1 mol of nitrogen reacts with 3 mol of hydrogen, 92 kJ of heat will be absorbed by the system.
C When 1 mol of ammonia reacts, 46 kJ of heat will be absorbed from the surroundings.
D When 2 mol of ammonia decomposes, the temperature will decrease by 92°C.

Short-answer questions

1 Write a balanced molecular equation for each of the following reactions.

a aluminium is heated with water vapour to give hydrogen gas and solid aluminium oxide
b chlorine gas is bubbled through a solution of sodium iodide to form solid iodine and a solution of sodium chloride
c solid manganese(IV) oxide (MnO_2) is added to dilute hydrochloric acid to produce water, chlorine gas and a solution of manganese(II) chloride
d solutions of calcium hydroxide and phosphoric acid are mixed to give a precipitate of calcium phosphate and water
e copper(II) oxide reacts with ammonia gas to produce copper, nitrogen gas and water

2 A sample of aluminium nitrate ($Al(NO_3)_3$) has a mass of 30.5 g.

a Calculate the amount, in mol, of aluminium nitrate in the sample.
b Calculate the amount, in mol, of nitrogen atoms present.
c Calculate the total number of atoms present in the sample.
d Determine the percentage by mass of oxygen in aluminium nitrate.

3 Copper forms two oxides, copper(I) oxide (Cu_2O) and copper(II) oxide (CuO). The following experiment was carried out to determine whether a particular oxide of copper was Cu_2O or CuO.

A sample of the oxide was dissolved in sulfuric acid. An excess of zinc powder was added to precipitate the copper as copper metal. The copper metal was collected, washed, thoroughly dried and then weighed. The results are given below:

m(oxide) = 2.127 g
m(dried copper) = 1.704 g

a Determine the empirical formula of this oxide of copper.
b If the sample analysed was a mixture of the two oxides instead of one of the oxides only, determine if the mass of copper obtained would be greater or less than 1.704 g. Explain your answer.

4 Marble chips (calcium carbonate) dissolve readily in hydrochloric acid to produce calcium chloride, carbon dioxide and water. The equation for this reaction is:

$$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$$

a Calculate the expected mass of carbon dioxide produced by the complete reaction of 2.75 g of marble chips.
b Calculate the percentage yield if the mass of carbon dioxide produced was 0.89 g.
c Suggest one reason why the mass of carbon dioxide obtained was less than the value calculated in part **a**.

5 The specific heat capacities of some common substances are listed in the table below.

Substance	Specific heat capacity ($J\,g^{-1}\,°C^{-1}$)
water	4.18
ethanol	2.4
copper	0.39

a Calculate the amount of heat energy, in J, required to increase the temperature of 250.0 g of water from 18°C to 100°C.
b Calculate the amount of energy required to raise the temperature of an equal mass of copper by the same amount.
c If the same amount of energy as in part **b** is used to heat 250.0 g ethanol, determine the temperature rise of the ethanol.
d Explain why water has a high heat capacity.
e Give one use for water based on its high heat capacity.

6 The specific heat capacity of water is $4.18\,J\,g^{-1}\,°C^{-1}$ and the specific heat capacity of liquid hexane (C_6H_{14}) is $2.29\,J\,g^{-1}\,°C^{-1}$.

a State what is measured by the specific heat capacity of a substance.

b A 100 g sample of water and 100 g of hexane are both at a temperature of 20.0°C. The same amount of heat is applied to each liquid. The temperature of the water rises to 32.0°C. Calculate the temperature the hexane rises to after heating.

7 Use the average bond enthalpies provided to calculate the enthalpy change for the following reaction. Indicate if the reaction is exothermic or endothermic. Explain your reasoning.

$$N_2(g) + 3Cl_2(g) \rightarrow 2NCl_3(g)$$

Bond	Average bond enthalpy ($kJ\,mol^{-1}$)
N = N	945
Cl–Cl	242
N–Cl	192

8 Butane undergoes combustion with oxygen according to the equation:

$$2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(l)$$
$$\Delta H = -5774\,kJ$$

Calculate the mass of butane gas needed to bring 500.0 mL of water to its boiling point if the initial temperature of the water was 23.0°C.

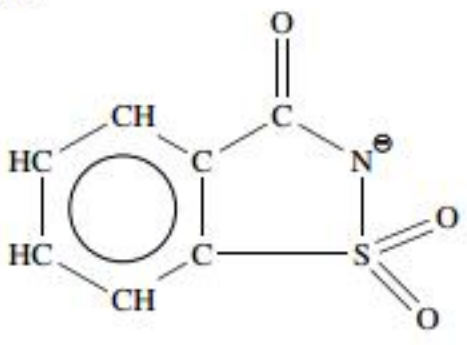
9 Ammonium sulfate and calcium hydroxide react in accordance with the following equation:

$$(NH_4)_2SO_4(s) + Ca(OH)_2(s) \rightarrow CaSO_4(s) + 2NH_3(g) + 2H_2O(l)$$

A mixture of 109 g of ammonium sulfate and 53.0 g of calcium hydroxide is gently heated, causing the reaction to occur.

Calculate the mass of ammonia produced.

10 A liquid sweetener contains the artificial sweetener calcium saccharin. The negative ion of saccharin is shown below.



To determine the percentage, by mass, of calcium saccharin in the liquid sweetener, 52.4 g of the liquid sweetener was completely converted to saccharin ions and sulfate ions.

A solution of barium chloride was then added to form an insoluble solid called barium sulfate, from all the sulfate ions. The insoluble barium sulfate solid was filtered from the mixture, dried and weighed. Its mass was 1.27 g.

a Determine the formula of calcium saccharin.

b Calculate the amount, in moles, of barium sulfate formed from the liquid sweetener.

c Calculate the amount, in moles, of sulfur atoms contained in this amount of barium sulfate.

d Assuming all the sulfur atoms in the barium sulfate were originally present in the calcium saccharin, calculate the mass of calcium saccharin in the 52.4 g sample of the liquid sweetener.

e Calculate the percentage, by mass, of calcium saccharin in the liquid sweetener.

11 A white crystalline solid of molecular formula $C_xH_yO_z$ was isolated from certain fruits and found to have a relative molecular mass of 180.

A 0.270 g sample of this solid was burnt to completion in air and produced 0.400 g of carbon dioxide and 0.160 g of water. Assume that all the carbon in the compound was converted to CO_2 and that all the hydrogen was converted to H_2O.

a Calculate the masses of carbon, hydrogen and oxygen present in the compound.

b Determine the empirical formula of the compound.

c Determine the molecular formula of the compound.

12 Hydrated salts have a set number of water molecules per unit formula incorporated into their crystal structure. One example of a hydrated salt is copper sulfate pentahydrate, $CuSO_4.5H_2O$. The water molecules, known as water of crystallisation, can be driven off by heating the hydrated salt.

$$CuSO_4.5H_2O(s) \rightarrow CuSO_4(s) + 5H_2O(g)$$

The product does not contain any water of crystallisation and is known as anhydrous copper sulfate.

Outline a procedure you would use to experimentally determine the number of water molecules per unit formula of hydrated barium chloride, which can be represented as $BaCl_2.xH_2O$.

The following information should be included in your description:

- a list of equipment and chemicals to be used
- a diagram showing the arrangement of the equipment
- steps in the experimental procedure
- a results table to record any measurements that are to be made
- an outline of the steps you would take to calculate the extent of hydration represented by *x* in the above formula.

13 A compound of antimony, antimony sulfide, is used to make safety matches. A small amount of antimony sulfide is mixed with potassium chlorate and glued to the tip of the matchstick. When the match is struck on the side of the matchbox, the red phosphorus on the side of the box ignites, which in turn ignites the antimony sulfide/potassium chlorate mixture. Heat from this reaction then makes the match wood burn.

a Predict the formulas of antimony sulfide (which contains the Sb^{3+} ion) and potassium chlorate.

b When antimony sulfide and potassium chlorate react, they form antimony oxide, potassium chloride and sulfur dioxide. Write a balanced equation for this reaction.

c Deduce if the reaction is endothermic or exothermic. Explain how you decided your answer.

d Sketch an energy profile diagram for the reaction of antimony sulfide with potassium chlorate, indicating the relative potential energies of the reactants and products and the activation energy.

14 The density of a liquid was determined by finding the mass of a measured volume of the liquid in a flask. The following results were obtained.

mass of flask = 30.00 ± 0.01 g

mass of flask + liquid = 46.00 ± 0.01 g

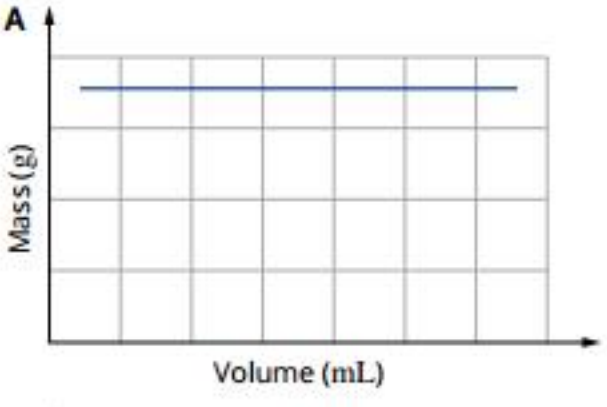
volume of liquid = 20.0 ± 0.2 mL

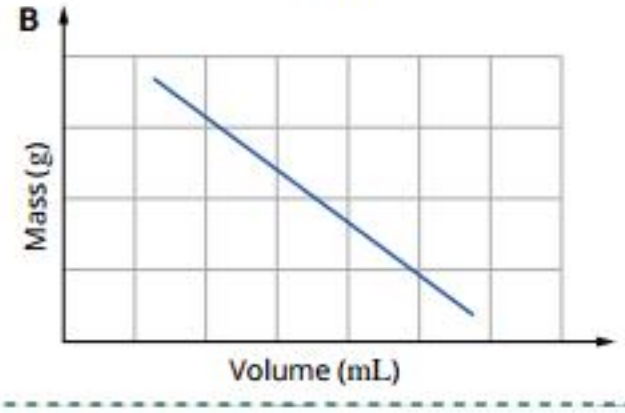
a Use the data provided to calculate the density of the liquid and its uncertainty.

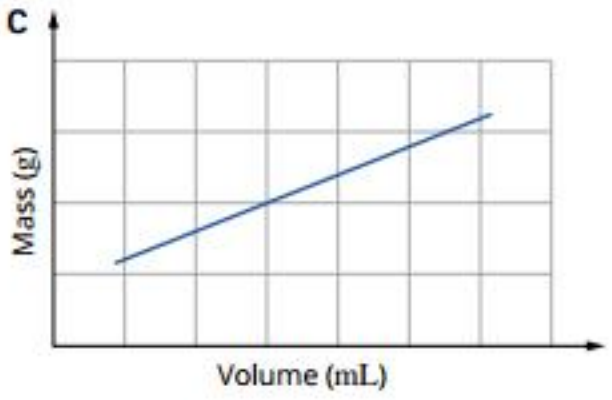
$$\text{density} = \frac{\text{mass}}{\text{volume}}$$

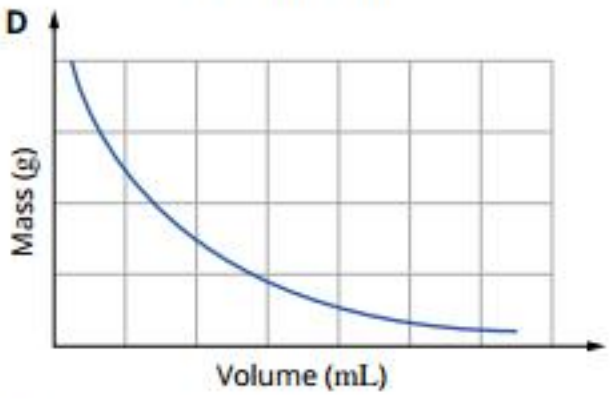
b The mass of different volumes of the same liquid were measured. The results were plotted on a graph using a line of best fit.

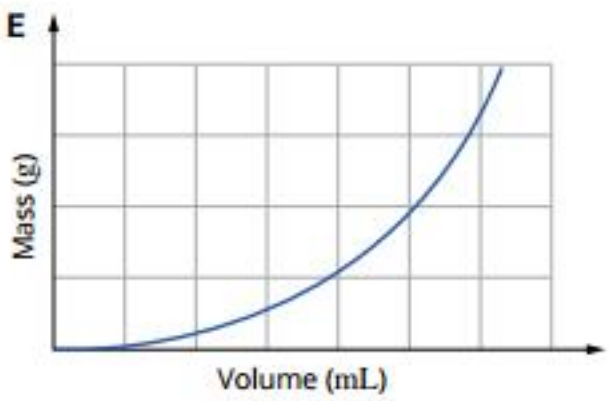
Select the graph that correctly represents the relationship between volume and mass of the liquid. Justify your selection.







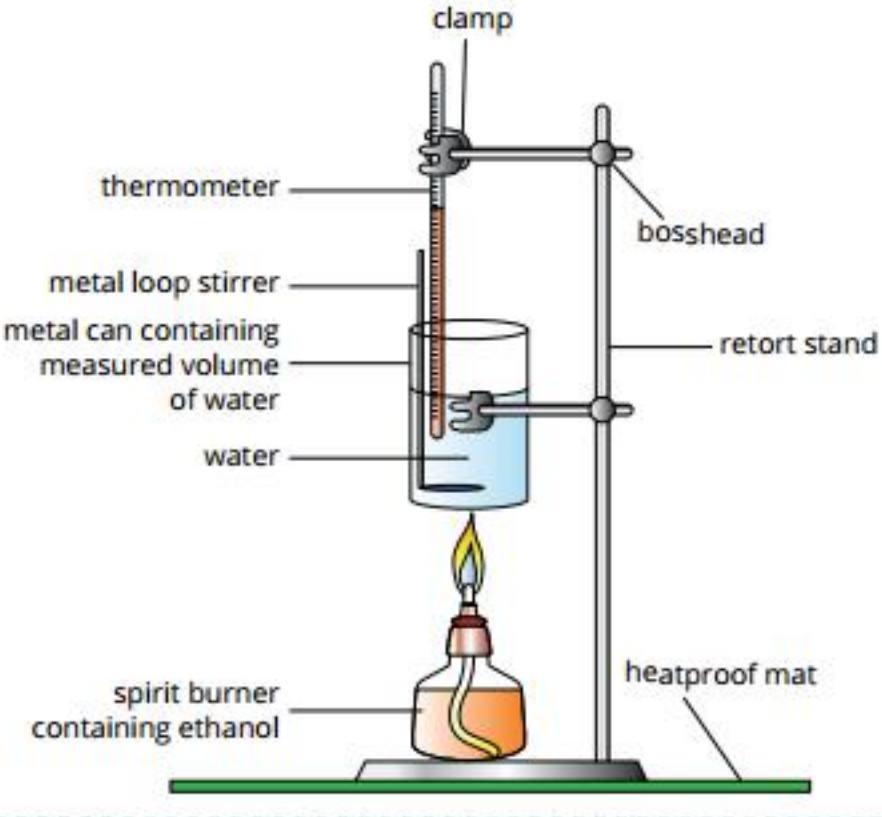




c Describe the data gathered in this experiment as either qualitative or quantitative. Explain your answer.

d Explain why analytical chemists aim to produce a set of measurements that are both accurate and precise.

15 The heat of combustion of ethanol, CH_3CH_2OH, was experimentally determined using the apparatus shown below.



The measurements taken in this experiment are provided below.

initial mass of burner and ethanol = 18.615 g
final mass of burner and ethanol = 18.298 g
volume of water = 200.0 mL
initial temperature of water = 21.34°C
final temperature of water = 31.97°C

The following information is also provided.

specific heat of water = 4.18 J g^{-1} $°C^{-1}$
density of water = 1.00 g mL^{-1}

a Use the experimental data provided to calculate the enthalpy of combustion of ethanol. Express your answer to an appropriate number of significant figures.

b Deduce if the combustion reaction is endothermic or exothermic. Explain your answer in terms of the experimental evidence.

c Discuss the endothermic or exothermic nature of the reaction in terms of bond energies.

d Use the enthalpy value calculated in part **a** above to write a thermochemical equation for the combustion reaction of ethanol.

e The value for the heat of combustion of ethanol quoted in chemical databases is 1367 kJ mol^{-1}.

i Calculate the percentage experimental error of the enthalpy value determined by this experiment.

ii Suggest one cause of this error and indicate how the experimental design could be improved.

iii Does the cause of the error identified in part **ii** produce a random or systematic error? Explain your decision.

f In this experiment, a change in temperature was used to calculate the heat energy released by a reaction. Explain the difference between heat and temperature.

16 A 50.0 mL water sample is known to contain barium ions (present as Ba^{2+}).

0.200 g of magnesium sulfate is added to precipitate the barium ions as barium sulfate. The precipitate is dried and weighed. Its mass is 0.126 g.

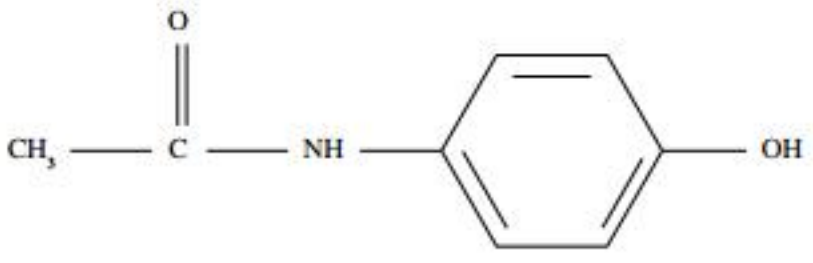
a Write a balanced equation for the reaction occurring.

b Determine the mass of barium in the original sample.

c Verify that the barium ions are the limiting reagent in the reaction with magnesium sulfate.

d The mass of magnesium sulfate added was found to be 0.220 g rather than 0.200 g. Explain how this error would impact the experimental result.

17 Paracetamol ($C_8H_9NO_2$) is a medicine used to treat mild pain. Its structure is shown below.



A pharmacy has a supply of 250 packets of paracetamol ($C_8H_9NO_2$). Each packet contains 20 tablets, with each tablet containing 500 mg of paracetamol.

a Calculate the total mass of paracetamol in the supply.

b Determine the mass of each element in the supply.

c Calculate the number of moles of carbon in the supply.

d Determine the total number of atoms in the supply.

18 A 2.80 g sample of an unlabelled compound is analysed and the mass of carbon is found to be 2.40 g. The remainder of the sample is hydrogen.

a Determine the empirical formula of the compound.

b The molar mass of the compound is 56 g mol^{-1}. What is the molecular formula of the compound?

c How many moles of this compound were in the original sample?

d Write a balanced equation for the combustion reaction between this substance and oxygen. The products are CO_2 and H_2O.

19 A 224 L domestic hot water system, running on natural gas, is filled with water at 14°C and requires combustion of 1.25 kg of fuel to heat the water to the storage temperature of 70°C. The density of water is 1.00 g mL^{-1}.

a Assuming 100% conversion, calculate the energy content, in MJ kg^{-1}, of the natural gas.

b A typical energy value for natural gas is 54 MJ kg^{-1}. Explain any difference between this value and your answer to part **a**.

20 A polystyrene cup containing 200 mL of black coffee is heated from 20°C to 100°C in a microwave oven operating at a power level of 1200 W. A power of 1 W (watt) is equivalent to an energy consumption of 1 J s^{-1}. Assume that there is no heat loss and that the density of the coffee solution is the same as water. Calculate the time required to heat the coffee to 100°C.

21 A Bunsen burner is used to heat a beaker containing 250.0 g of water. Complete combustion of 0.0303 mol of methane raises the temperature of the water from 21.0°C to 39.2°C. The thermochemical equation for the combustion of methane is:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$$
$$\Delta H = -890 \text{ kJ mol}^{-1}$$

Calculate the percentage of the Bunsen burner's energy that is lost to the environment.

UNIT 2 Molecular interactions and reactions

TOPIC 1 Intermolecular forces and gases

TOPIC 2 Aqueous solutions and acidity

TOPIC 3 Rates of chemical reactions

Unit 2 objectives

- Describe ideas and findings about intermolecular forces and gases, aqueous solutions and acidity, and rates of chemical reactions
- Apply understanding of intermolecular forces and gases, aqueous solutions and acidity, and rates of chemical reactions
- Analyse data about intermolecular forces and gases, aqueous solutions and acidity, and rates of chemical reactions
- Interpret evidence about intermolecular forces and gases, aqueous solutions and acidity, and rates of chemical reactions
- Evaluate processes, claims and conclusions about intermolecular forces and gases, aqueous solutions and acidity, and rates of chemical reactions
- Investigate phenomena associated with intermolecular forces and gases, aqueous solutions and acidity, and rates of chemical reactions

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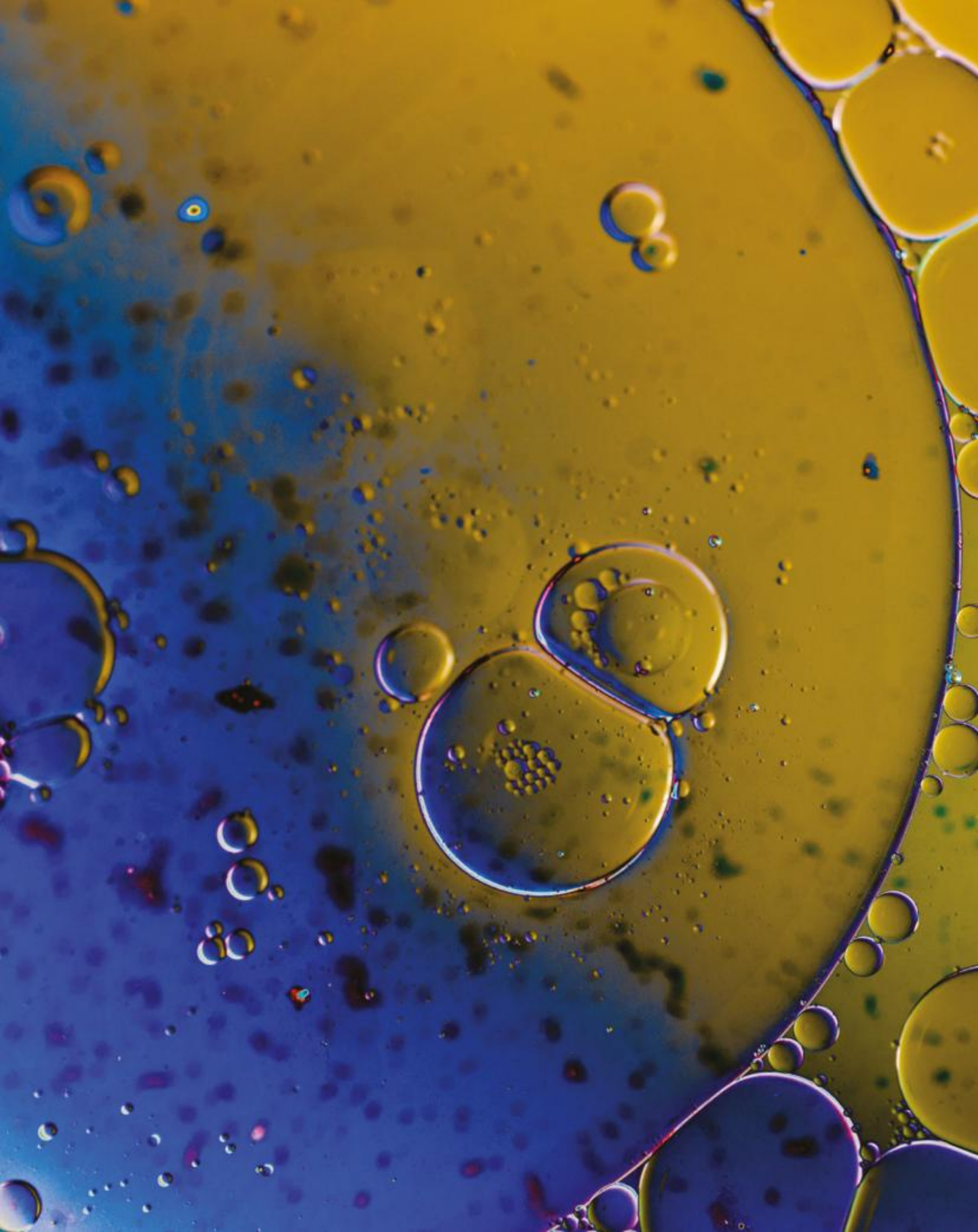

CHAPTER

11 Intermolecular forces and chromatography

Covalent molecular substances have a much greater range of properties than ionic or metallic substances. Covalent molecular substances are the only substances that can be solids, liquids or gases at room temperature. They can be hard or soft, flexible or brittle, sticky or oily—almost any consistency. This broad range of properties makes molecular substances very useful materials.

The properties of covalent molecular substances can generally be explained by the strong covalent bonds within the molecules (intramolecular bonds) and the much weaker forces of attraction between the molecules (intermolecular forces).

During this chapter, you will become familiar with the valence shell electron pair repulsion (VSEPR) theory and use it to predict the shape and polarity of molecules. Knowing the shapes of molecules and whether or not they are polar is vital when predicting and explaining the type and strength of intermolecular forces acting between the molecules.

You will learn to identify intermolecular forces including dipole–dipole forces, hydrogen bonding and dispersion forces, and consider factors that influence the strength of these forces. These intermolecular forces determine many of the physical properties of covalent molecular substances including vapour pressure, melting and boiling points, and solubility. Finally, you will use your understanding of intermolecular forces and solubility to understand two analytical techniques, paper chromatography and thin-layer chromatography. These methods separate and identify components of a mixture.

Syllabus subject matter

Topic 1 • Intermolecular forces and gases

INTERMOLECULAR FORCES

- Apply the valence shell electron pair repulsion (VSEPR) theory to determine the shape and bond angles of linear, bent, trigonal planar, tetrahedral and pyramidal molecules. (Hybridization involving d-orbitals are not required.) **11.1**
- Determine the polarity of molecules using molecular shape, understanding of symmetry, and comparison of the electronegativity of elements. **11.2**
- Explain the relationship between vapour pressure, melting point, boiling point and solubility, and the nature and strength of intermolecular forces (e.g. dispersion forces, dipole–dipole attractions, and hydrogen bonding) within molecular covalent substances. **11.3, 11.4**

CHROMATOGRAPHY TECHNIQUES

- Identify that paper and thin-layer chromatography can be used to determine the composition and purity of substances. **11.5**
- Explain how variations in the strength of the interactions between atoms, molecules or ions in the mobile and stationary phases can be used to separate components. **11.5**
- Analyse paper and thin-layer chromatographs to determine the composition and purity of substances, including calculating R_f values. **11.5**

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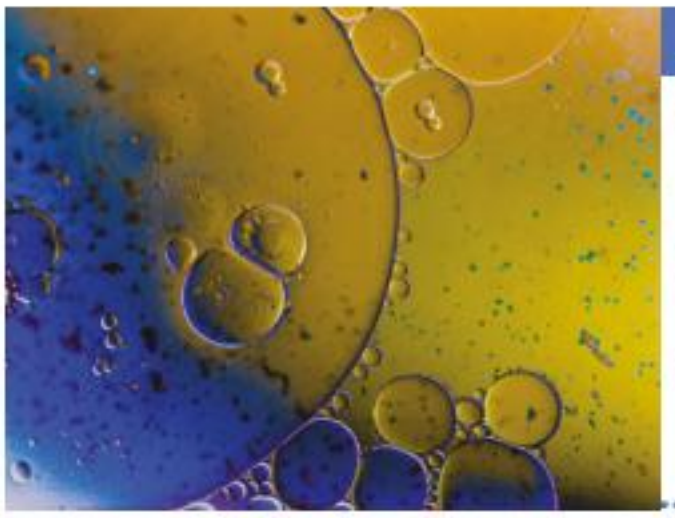
11.1 Valence electron pair arrangement and molecular shape



BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that the valence shell electron pair repulsion (VSEPR) theory assumes the valence shell electron pairs around atoms in a molecule are arranged to minimise repulsion between electron pairs
- apply VSEPR theory in conjunction with Lewis structures to determine valence electron pair arrangement and shapes of molecules
- understand how the presence of lone pairs of electrons affects a molecule's bond angles and be able to deduce the approximate bond angles between atoms in various molecules.

FIGURE 11.1.1 Water (H_2O) molecules have a distinctive shape that is responsible for many of water's properties. The valence shell electron pair repulsion theory accurately predicts the shape of water molecules.

The shapes of molecules are critical in determining many physical properties of covalent molecular substances. In particular, molecular shape affects vapour pressure, melting point, boiling point and solubility. This is because the shape of a molecule (along with electron distribution throughout the molecule) determines how it interacts with other molecules.

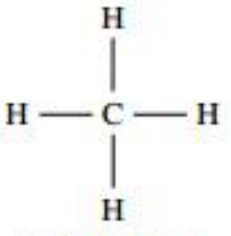
For very large molecules, such as DNA, proteins and enzymes, shape plays a key role in how they behave chemically and biologically. For example, the twisted double helix of DNA allows the molecule to coil up tightly so that it fits inside the nucleus of a cell. To understand the shape of large molecules like DNA, scientists use complex techniques such as X-ray crystallography or powerful computer simulations. However, the shape of small molecules can be predicted using a relatively simple model known as the **valence shell electron pair repulsion (VSEPR) theory**. In this module, you will see how VSEPR theory can be used to predict the shapes of molecules such as the water molecule represented in Figure 11.1.1.

VALENCE SHELL ELECTRON PAIR REPULSION THEORY

As the name suggests, VSEPR theory uses our knowledge of the **valence electrons** in the atoms of a molecule to predict the shape of the molecule. VSEPR theory is based on the principle that negatively charged electron pairs, both **bonding pairs** and **lone pairs**, in the valence shell of an atom repel each other. As a consequence, these electron pairs are arranged as far away from each other as possible. The arrangement of valence electron pairs (bonding pairs and lone pairs) around the central atom of a molecule is called its geometry, or its **electron pair arrangement**.

Molecules with four electron pairs around the central atom

In Chapter 8, you saw that atoms in covalent molecules are generally most stable when they have eight electrons in their valence shell. This is known as the **octet rule**. These eight electrons are arranged into four pairs of electrons.



Lewis structure

FIGURE 11.1.2 This Lewis structure of a methane (CH_4) molecule is made up of four C–H covalent bonds. Each covalent bond represents a pair of bonding electrons (there are no lone pairs).

For example, consider the **Lewis structure** of the methane molecule shown in Figure 11.1.2 in which the carbon atom is covalently bonded to four hydrogen atoms. Each covalent bond represents a pair of electrons that the carbon atom shares with a hydrogen atom; the four pairs of electrons give the carbon atom a stable octet. There are no lone pairs. Note that hydrogen is an exception to the octet rule as the $n = 1$ shell can only accommodate a maximum of two valence electrons. Each of the four hydrogen atoms in methane shares one pair of electrons with the carbon atom to give them the same electron configuration as helium, a very stable gas.

As discussed in Chapter 8, Lewis structures are often used to simplify the drawing of molecules. In a Lewis structure, lines are used to represent the two electrons in a covalent bond. One line represents one pair of **bonding electrons**.

VSEPR theory dictates that the electron pairs repel each other so that they are as far apart as possible. In methane, there are four **bonding pairs** of electrons that make up the four C–H covalent bonds. The repulsion between these four pairs of electrons results in a three-dimensional **tetrahedral** electron pair arrangement around the central carbon atom as shown in the ball and stick model in Figure 11.1.3. The tetrahedral electron pair arrangement ensures that the electron pairs are as far from each other as possible with angles of 109° between all of the single bonds.

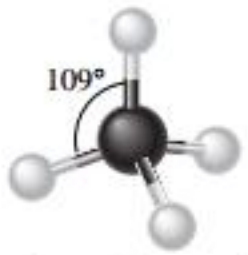


FIGURE 11.1.3 In a methane molecule (CH_4), the electron pairs in the single covalent bonds repel each other. The repulsion forces the bonds as far apart as possible, leading to a tetrahedral molecular shape with bond angles of 109°.

Lone pairs of electrons

Bonding pairs of electrons form the covalent bonds within a molecule. However, not all electron pairs are involved in bonding. Some electrons form a **lone pair of electrons**, also called a non-bonding pair. In VSEPR theory, lone pairs are treated in the same way as bonding pairs of electrons in terms of predicting the positioning of these electron pairs around the central atom.

In the ammonia molecule shown in Figure 11.1.4, the nitrogen atom has a stable octet made up of three bonding pairs of electrons (which form three covalent N–H bonds) and one lone pair of electrons. These four pairs of electrons repel each other to give a tetrahedral electron pair arrangement around the central atom. It is important to understand that VSEPR theory uses both lone pairs and bonding pairs of electrons to determine the electron pair arrangement and the angles between them. However, the shape of the molecule is derived by considering only the position of the bonding pairs (in other words, the position of the atoms). Therefore, in the case of ammonia, while the electron arrangement is tetrahedral, the lone pair is ignored when determining the shape of the molecule, which is **pyramidal**. The lone pair of electrons occupies slightly more space than the bonding electrons. This results in greater repulsion from the lone pairs; therefore, the covalent bonds between the nitrogen atom and the three hydrogen atoms are pushed closer together. The **bond angles** are 107°, which is slightly less than the 109° in methane.

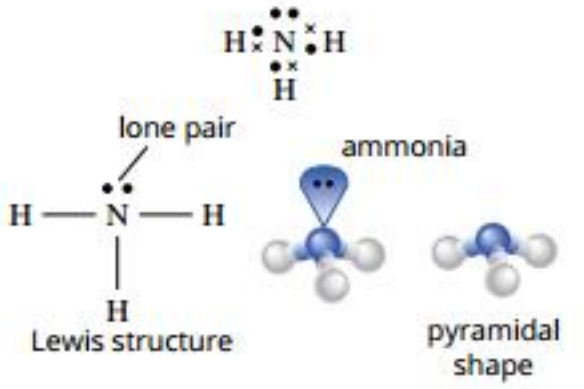


FIGURE 11.1.4 The Lewis structure of an ammonia (NH_3) molecule shows that the nitrogen atom has a total of four pairs of electrons: three bonding pairs (which form the three covalent bonds) and one lone pair. Therefore, the electron arrangement around the nitrogen atom is tetrahedral, due to the repulsion of all four electron pairs, but the molecular shape is pyramidal.

In the water molecule shown in Figure 11.1.5, the oxygen atom has a stable octet made up of two bonding pairs of electrons (which form two covalent O–H bonds) and two lone pairs. In total, there are four pairs of electrons that repel each other to give a tetrahedral electron pair arrangement. To determine the shape of the molecule, the two lone pairs of electrons are ignored and the shape is described as bent. With two lone pairs in the molecule, the two single covalent bonds are pushed closer together. The bond angle around the central oxygen atom is 104.5°, which is slightly less than the 107° in ammonia, and demonstrates the effect of the extra repulsion from the second lone pair of electrons.

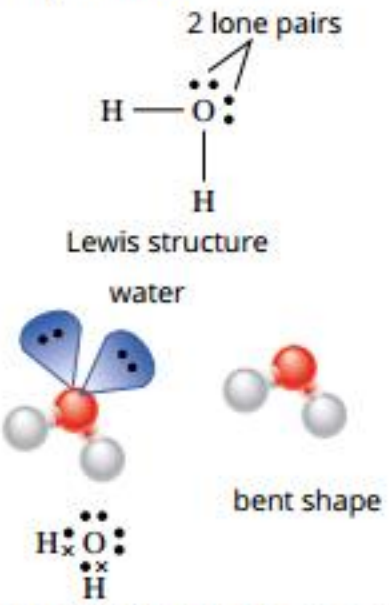


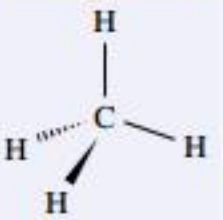
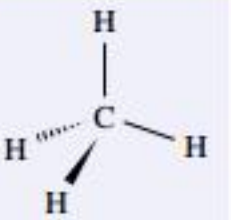
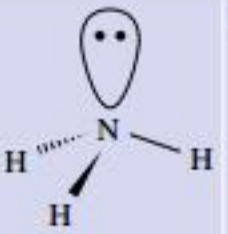
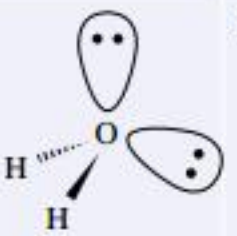
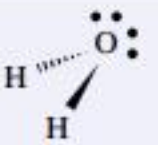
FIGURE 11.1.5 The Lewis structure of a water (H_2O) molecule shows that the oxygen atom has a total of four pairs of electrons: two bonding pairs (which form the two covalent bonds) and two lone pairs. Therefore, the electron arrangement around the oxygen atom is tetrahedral, due to the repulsion of all four electron pairs, but the shape of the molecule is bent.

Electron pair arrangement is determined by considering all electron pairs (bonding and lone) in the valence shell of the central atom of a molecule.

In contrast, the shape of the molecule is determined by considering the arrangement of bonded atoms relative to each other and therefore does not consider lone pairs.

In Table 11.1.1, the electron arrangement, shapes and bond angles of methane, ammonia and water are compared. Note that the structures of each molecule in the table are drawn using the **wedge-dash notation** to show the three-dimensional arrangement of the atoms. Using this notation, bonds drawn with lines are in the plane of the page, bonds drawn with bold wedges are coming out of the page towards you, and bonds drawn with dashed lines are going away from you, behind the page. You can see that the methane, ammonia and water molecules all have a tetrahedral electron pair arrangement but the shape of each molecule depends on the positions of the bonded atoms. You can also see that the bond angles decrease as the number of lone pairs of electrons around the central atom increases; the lone pairs occupy slightly more space than the bonding electrons and push the covalently bonded atoms closer together.

TABLE 11.1.1 A comparison of electron pair arrangement, molecular shape and bonding angles in methane, ammonia and water

Molecule	Total pairs of electrons on central atom	Electron pair arrangement	Bonding pairs	Lone pairs	Molecular Shape	Bond angles (°)
methane	4	 tetrahedral	4	0	 tetrahedral	109
ammonia	4	 tetrahedral	3	1	pyramidal	107
water	4	 tetrahedral	2	2	 bent	104.5

Lone pairs of electrons occupy more space than bonding electrons and change the bond angles in the molecule.

In a hydrogen fluoride molecule, the fluorine atom has a stable octet made up of one bonding pair of electrons (which forms the covalent H–F bond) and three lone pairs. In total, there are four pairs of electrons surrounding the fluorine atom that repel each other to give a tetrahedral electron pair arrangement. To determine the shape of the molecule, the three lone pairs of electrons are ignored and the shape is described as linear, as shown in Figure 11.1.6.

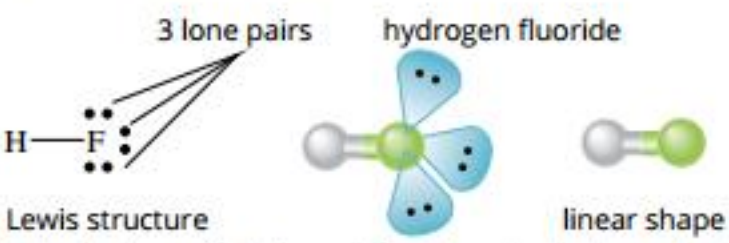
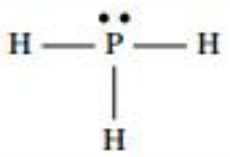


FIGURE 11.1.6 The Lewis structure of a hydrogen fluoride molecule shows that the fluorine atom has a total of four pairs of electrons: one bonding pair (which forms the covalent bond) and three lone pairs. Therefore, the geometry of electron pairs around the fluorine atom is tetrahedral, due to the repulsion of all four electron pairs, but the shape of the molecule is linear.

Worked example 11.1.1

PREDICTING THE SHAPE OF MOLECULES

Predict the shape of a molecule of phosphine (PH_3).	
Thinking	**Working**
Draw the Lewis structure for the molecule.	
Count the number of bonding pairs and lone pairs of electrons on the central atom and determine the total number of electron pairs.	There are three bonding pairs and one lone pair—a total of four pairs of electrons.
Determine how the pairs of electrons will be arranged to get maximum separation.	The four pairs of electrons will be distributed in a tetrahedral electron pair arrangement.
Deduce the shape of the molecule by ignoring the lone pairs and considering the arrangement of just the atoms.	The shape of the molecule is pyramidal.

➤ Try yourself 11.1.1

PREDICTING THE SHAPE OF MOLECULES

Predict the shape of a molecule of hydrogen sulfide (H_2S).

Molecules with fewer than four electron groups around the central atom

As discussed above, the shape of a molecule is determined by considering the repulsion between regions of high electron density around a central atom. VSEPR theory can also be applied to molecules in which the central atom forms multiple bonds (double and triple bonds) and therefore has fewer regions of electron density around the nucleus.

A double bond contains two pairs of electrons. A triple bond contains three pairs of electrons. VSEPR theory treats double and triple bonds in the same way that it treats single bonds. A double and triple bond are both considered to be one group of bonding electrons and the effect is the same as a pair of electrons in a single bond.

For example, consider the molecule in Figure 11.1.7. This represents a molecule of methanal (which is more commonly known as formaldehyde) and has the formula CH_2O. The central carbon atom has a stable octet made up of four pairs of bonding electrons. However, there are only three groups of electrons surrounding the carbon atom as the double bond (which is made up of two pairs of bonding electrons) counts as one group. These three groups of electrons repel each other to get maximum separation and are distributed in a **trigonal planar** electron pair arrangement. Furthermore, because there are no lone pairs of electrons surrounding the central carbon atom, the shape of the molecule is also trigonal planar because the atoms form a triangle in one plane. Trigonal planar molecules have bond angles of 120°.

FIGURE 11.1.7 Methanal (also called formaldehyde) has a central carbon atom that forms a double bond with an oxygen atom and single bonds with two hydrogen atoms. The three groups of electrons repel each other to form a trigonal planar geometry of electron groups around the central carbon atom. The shape of the molecule is also trigonal planar due to the absence of lone pairs around the central atom.

The central carbon atom in the carbon dioxide molecule shown in Figure 11.1.8 is surrounded by four pairs of bonding electrons. However, there are only two groups of electrons as each double bond (which is made up of two bonding pairs of electrons) counts as one group. The two groups of electrons repel each other to get maximum separation. Since there are no lone pairs of electrons surrounding the central carbon atom, the molecule is linear. Linear molecules have bond angles of 180°.

carbon dioxide, CO_2
(linear)

FIGURE 11.1.8 In a carbon dioxide molecule, the carbon atom forms double bonds with two oxygen atoms. The two groups of electrons repel each other to form a linear geometry of electron groups around the central carbon atom. The shape of the molecule is also linear due to the absence of lone pairs around the central atom.

Another example of a linear molecule in which the central atom has a multiple bond is hydrogen cyanide (HCN), as shown in Figure 11.1.9. In this molecule, the central carbon atom has a single bond to the hydrogen atom and a triple bond to the nitrogen atom. Like the double bonds in carbon dioxide, the triple bond between carbon and nitrogen is treated as one group of electrons so that overall there are only two groups of electrons surrounding the central atom. This results in a linear geometry of electron groups around the central carbon atom and also a linear shape, since there are no lone pairs on the central atom.

hydrogen cyanide, HCN
(linear)

FIGURE 11.1.9 The hydrogen cyanide molecule is linear. In this case, the central carbon atom forms a triple bond with the nitrogen atom and a single bond with the hydrogen atom.

Double and triple bonds count as one group of electrons.

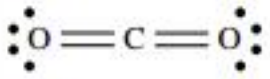
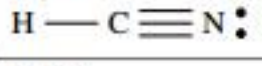
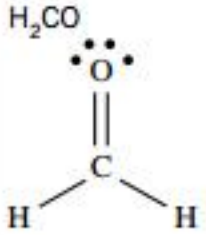
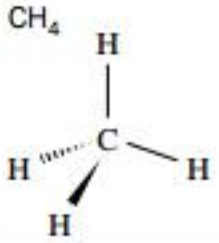
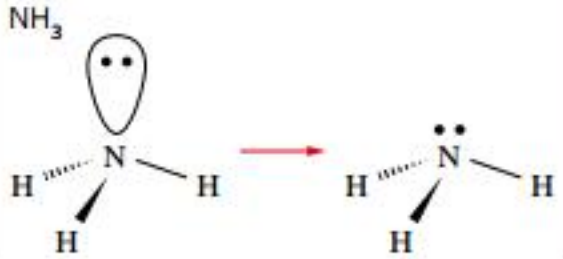
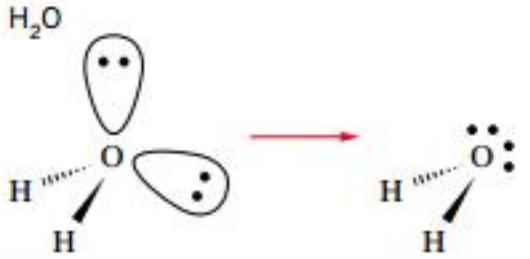
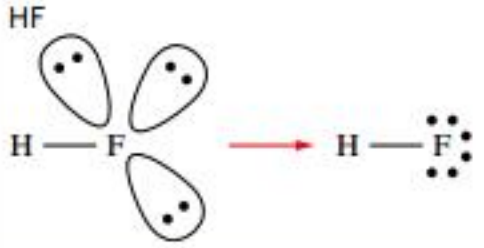
VSEPR theory can be explored further through the practical investigation on page 476.

11.1 Review

SUMMARY

- The shapes of simple molecules can be predicted by the valence shell electron pair repulsion (VSEPR) theory, as shown in Table 11.1.2.
- VSEPR theory is based on the principle that electron pairs in the valence shell of an atom repel each other. When applied, VSEPR theory predicts that these electron pairs are arranged as far away from each other as possible.
- Electron pairs can exist as bonding electrons (in covalent bonds) or as lone pairs of electrons.
- Lone pairs of electrons and bonding electrons repel each other due to the repulsion between clouds of negative charge.
- Lone pairs affect the bond angles in a molecule but are not considered when describing the shape of the molecule.
- Double and triple bonds count as one electron group when determining the electron arrangement around the central atom.

TABLE 11.1.2 Summary of shapes of molecules

Total electron groups	Electron pair arrangement	Bonding groups	Lone pairs	Molecular shape	Approximate bond angles (°)	Examples
2	linear	2	0	linear	180	CO_2 
						HCN 
3	trigonal planar	3	0	trigonal planar	120	H_2CO 
4	tetrahedral	4	0	tetrahedral	109	CH_4 
		3	1	pyramidal	107	NH_3 
		2	2	bent	104.5	H_2O 
		1	3	linear	180	HF 

11.1 Review *continued*

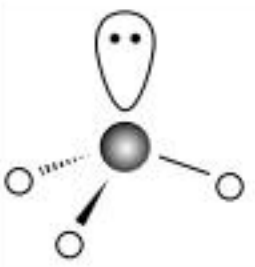
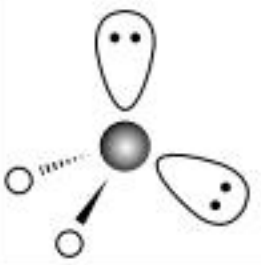
KEY QUESTIONS

Describe

1 **a** Identify what VSEPR stands for.
b Define a lone pair of electrons.
c Define a bonding pair of electrons.

Apply

2 Copy the table below and use VSEPR theory to identify the molecular shape in each case.

Molecule	Bonding groups	Lone pairs	Electron pair arrangement	Molecular shape
a	3	1		
b	2	2		
c	2	0		

3 Identify the electron pair arrangement of each of the structures shown in the table of Question 2. Explain any differences you note in the electron pair arrangement and the molecular shape.

4 Draw the Lewis structure and then use VSEPR theory to determine the shape of each of the following molecules.
a CF_4
b H_2Se
c CS_2

5 Determine the number of bonding pairs and lone pairs of electrons around the central atoms in each of the examples given in Question 4.

6 Explain the differences in bond angles in the methane (CH_4) and water (H_2O) molecules.

Analyse

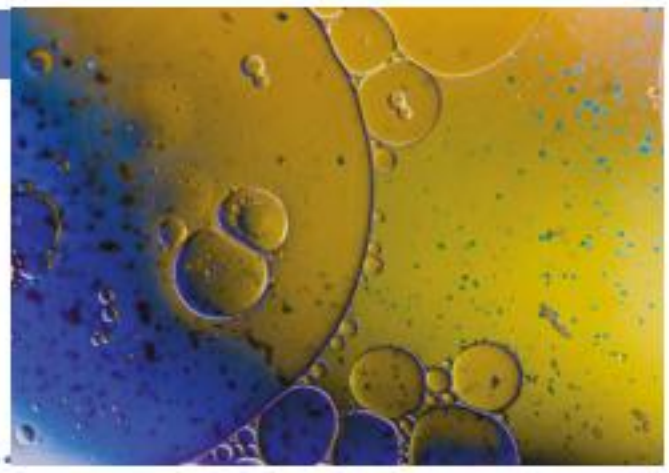
7 Identify which of the following would be expected to produce molecules with a pyramidal shape. Justify your choice.
H_2O NCl_3 CH_4 PH_3 SiO_2

8 Predict and explain the bond angles in $COCl_2$, CF_4 and CSe_2.

11.2 Polarity of molecules

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand the concept of electronegativity and that it is the key factor in determining electron distribution within molecules
- compare the electronegativity of different elements based on their positions in the periodic table
- use electronegativity to determine the polarity of diatomic molecules
- use electronegativity and molecular shape to determine the polarity of polyatomic molecules.



The shape of a molecule is critical in determining many physical properties of covalent molecular substances. In addition to the shape of the molecule, the **electron distribution** within a molecule is also critical to the physical properties of covalent molecules; the type and strength of the intermolecular forces between molecules depend strongly upon each molecule's shape and electron distribution.

Intermolecular forces are an example of **electrostatic forces**. You have already seen many other examples of how electrostatic forces form bonds at the atomic level. The attractions between positive and negative ions in an ionic crystal lattice (Chapter 7) and the attraction of shared electrons and nuclei in a covalent bond (Chapter 8) are examples of electrostatic forces.

The electrostatic attraction between molecules works in a similar way. An intermolecular force of attraction is the electrostatic attraction between the electrically positive regions in one molecule and the electrically negative regions in a neighbouring molecule. These unevenly charged regions are the result of uneven electron distributions within the molecules. In this module, you will examine how the shape of the molecule and the **electronegativity** of its atoms can cause these uneven electron distributions.

ELECTRONEGATIVITY AND POLARITY

Electronegativity is a key factor in determining the electron distribution in molecules. Electronegativity is the tendency of an atom in a covalent bond to attract electrons. Electronegativity increases from left to right across the periods of the periodic table and decreases down the groups of the table, as shown in Figure 11.2.1. You will remember seeing these patterns in Chapter 4.

Electronegativity increases

Electronegativity decreases

Period \ Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1						2.2 H												He
2	1.0 Li	1.6 Be											2.0 B	2.6 C	3.0 N	3.4 O	4.0 F	Ne
3	0.9 Na	1.3 Mg											1.6 Al	1.9 Si	2.2 P	2.6 S	3.2 Cl	Ar
4	0.8 K	1.0 Ca	1.4 Sc	1.5 Ti	1.6 V	1.7 Cr	1.6 Mn	1.8 Fe	1.9 Co	1.9 Ni	1.9 Cu	1.7 Zn	1.8 Ga	2.0 Ge	2.2 As	2.55 Se	3.0 Br	Kr
5	0.8 Rb	1.0 Sr	1.2 Y	1.3 Zr	1.6 Nb	2.2 Mo	2.0 Tc	2.2 Ru	2.3 Rh	2.2 Pd	2.0 Ag	1.7 Cd	1.8 In	2.0 Sn	2.0 Sb	2.1 Te	2.7 I	Xe
6	0.8 Cs	0.9 Ba																

2.2 H — electronegativity; symbol

FIGURE 11.2.1 Table of electronegativity values. This periodic table shows the electronegativities of the atoms of each element. The electronegativities increase from left to right across the periods and decrease down the groups.

The **polarity** of a covalent bond is a measure of the unequal sharing of electrons between the two atoms in the bond and is a result of the difference in the electronegativities of the bonded atoms. A diatomic molecule contains only one covalent bond, so its molecular polarity is simply determined by its bond polarity. However, the polarity of a polyatomic molecule depends not only on the individual bond polarities but also on how those individual bonds are arranged (i.e. the shape of the molecule).

Polarity of diatomic molecules

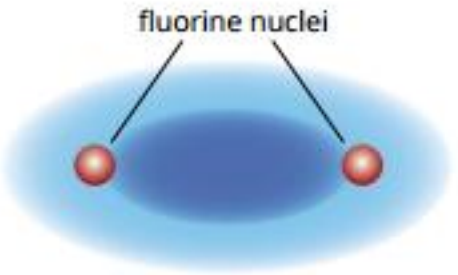
When two atoms form a covalent bond, you can regard the atoms as competing for the bonding electrons shared between them. The atom that has the stronger pull on the electrons is the one with the greater electronegativity.

Non-polar diatomic molecules

If the covalent bond is between atoms of the same element, then the atoms will have identical electronegativities and the electrons will be shared equally between them. This is the case for diatomic molecules of elements such as chlorine (Cl_2), oxygen (O_2), hydrogen (H_2) and nitrogen (N_2).

Bonds with an even distribution of valence (outer shell) electrons are said to be **non-polar** because there is no separation of charge at either end of the molecule.

Figure 11.2.2 shows the electron distribution in the non-polar fluorine molecule (F_2). The molecule has a high **electron density** between the two fluorine atoms, forming the covalent bond. However, the valence electrons are distributed evenly between the two atoms, making the bond non-polar.



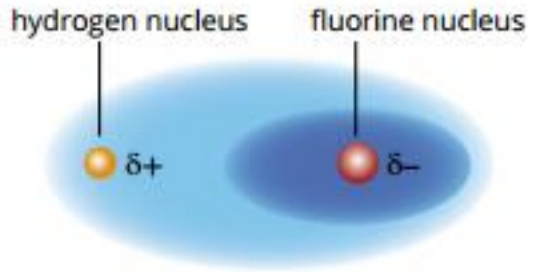
F_2 contains a non-polar bond.

FIGURE 11.2.2 Fluorine molecules have an even distribution of electrons and are therefore non-polar.

Polar diatomic molecules

If the covalent bond is between atoms of two different elements, then the electrons will stay closer to the more electronegative atom as it has a stronger pull on the electrons in the bond. An example is the hydrogen fluoride (HF) molecule, shown in Figure 11.2.3. Bonds with an uneven distribution of electrons are said to be **polar**.

A fluorine atom is more electronegative than a hydrogen atom. Therefore, in a hydrogen fluoride molecule the shared electrons tend to stay closer to the fluorine atom. This imbalance in the electron distribution means the fluorine atom is slightly negatively charged and the hydrogen atom is slightly positively charged. A molecule with oppositely charged poles is said to be polar. The fluorine atom is described as having a partial negative charge, which is represented with the Greek letter delta as δ–. The hydrogen atom is described as having a partial positive charge, δ+. The separation of these partial positive and negative charges is known as an **electric dipole**, or simply as a **dipole**, because there are oppositely charged poles at each end of the molecule. The diagram in Figure 11.2.4 shows the direction of the dipole using a crossed arrow pointing in the direction of the partial negative charge.



HF contains a polar bond; fluorine is more electronegative than hydrogen.

FIGURE 11.2.3 The electron distribution in hydrogen fluoride is uneven because of the different electronegativities of the hydrogen and fluorine atoms. Hydrogen fluoride is an example of a polar molecule.

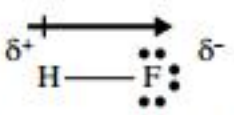


FIGURE 11.2.4 A representation of the dipole in hydrogen fluoride.

Hydrogen fluoride is polar because it has a permanent electric dipole created by the different electronegativities of the two atoms. All diatomic molecules that are made up of atoms with different electronegativities are polar to some extent. The level of polarity will depend on the difference in the electronegativities of the two atoms. The greater the difference, the greater the polarity of the molecule.

The partial charges on polar molecules are different from the charges on ions. The atom at the partially negative end of the bond can be considered as having a larger share of the electrons (or an excess of electrons). Conversely, the atom at the partially positive end of the bond can be considered as having lost some of its share of the electrons that would have balanced the positive charge of the protons. Consequently, this end is slightly 'naked' in terms of electrons—exposing the positive charge beneath. However, this charge separation is not complete—there are no electrons lost or gained as happens in the formation of ions. The partial charges on a polar molecule will always add to give a total charge of zero so the molecule will be neutral overall. The partial charges on a polar molecule are also a lot weaker than the charges on ions.

It is not just the covalent bonds in diatomic molecules that can be polar. Covalent bonds in larger molecules can have some degree of polarity. The polarity of any covalent bond can be compared by examining the difference in the electronegativities of the atoms involved in the bond.

Worked example 11.2.1

COMPARING THE POLARITY OF DIATOMIC MOLECULES

Compare the polarity of hydrogen fluoride (HF) and carbon monoxide (CO).	
Thinking	**Working**
Use the values in Figure 11.2.1 on page 273 to find the electronegativities of the atoms in each molecule.	HF: hydrogen 2.2; fluorine 4.0 CO: carbon 2.6; oxygen 3.4
For each molecule, subtract the lowest electronegativity value from the highest value.	HF: 4.0 – 2.2 = 1.8 CO: 3.4 – 2.6 = 0.8
Compare the electronegativity differences in both molecules; the more polar molecule has the biggest difference.	HF is more polar than CO.

As the difference in electronegativities of two atoms increases, the covalent bond formed between them increases in polarity.

➤ Try yourself 11.2.1

COMPARING THE POLARITY OF DIATOMIC MOLECULES

Compare the polarity of nitrogen monoxide (NO) and hydrogen chloride (HCl).

Polarity of polyatomic molecules

Determining the polarity of **polyatomic molecules** (those with more than two atoms) is a little more complicated. This is because the polarity of polyatomic molecules depends on the shape of the molecules as well as the polarity of the covalent bonds within the molecules. As a general rule:

- **symmetrical molecules** are non-polar
- **asymmetrical molecules** are polar.

In this context, when considering the diagrams that follow, it is useful to imagine that the electrons are being pulled towards the slightly negative end of the dipoles; then to consider whether the direction and magnitude of the individual dipoles would cancel each other out. If they do, the molecule would be classified as symmetrical and be non-polar (an analogy for this would be a dead heat in a 'tug-of-war' for electrons). If the dipoles are not cancelled out, then the molecule is considered asymmetrical and the molecule would have a **net dipole** (an uneven distribution of charge over the molecule as a whole) and be polar.

Electron density is the measure of the probability of an electron being present at a particular location within an atom.

Non-polar polyatomic molecules

As discussed above, even molecules with polar covalent bonds can be non-polar if the molecule is symmetrical.

Figure 11.2.5a on page 276 shows a molecule of methane in which the carbon atom is slightly more electronegative than the hydrogen atoms. Therefore, the carbon atom attracts the electrons more strongly than each hydrogen atom and has a partial negative charge, leaving hydrogen with a partial positive charge. However, the molecule has a perfect tetrahedral shape and is therefore symmetrical. The symmetry of the molecule means that the individual dipoles of the covalent bonds cancel each other perfectly (Figure 11.2.5b). The result is a molecule with no net dipole. Methane is an example of a non-polar molecule with slight polar covalent bonds (due to slight differences in electronegativities of C and H).

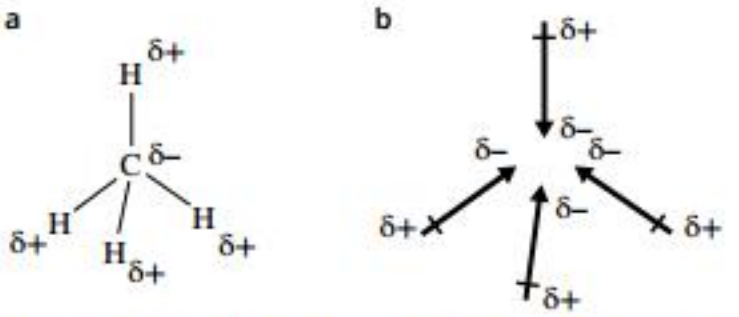


FIGURE 11.2.5 (a) Structure of a methane molecule showing the partial charges on the atoms. (b) The individual dipoles are distributed symmetrically around the molecule.

Polar polyatomic molecules

In asymmetrical molecules, the individual dipoles of the covalent bonds do not cancel each other. This results in a net dipole, making the molecule polar.

The chloromethane molecule shown in Figure 11.2.6a is an example of an asymmetrical molecule. The chlorine atom is more electronegative than the carbon atom. Therefore, the chlorine atom attracts electrons from the carbon atom while the carbon atom attracts electrons from the hydrogen atoms. The individual dipoles of the covalent bonds are shown in Figure 11.2.6b. These add to give the molecule a net dipole as shown in Figure 11.2.6c.

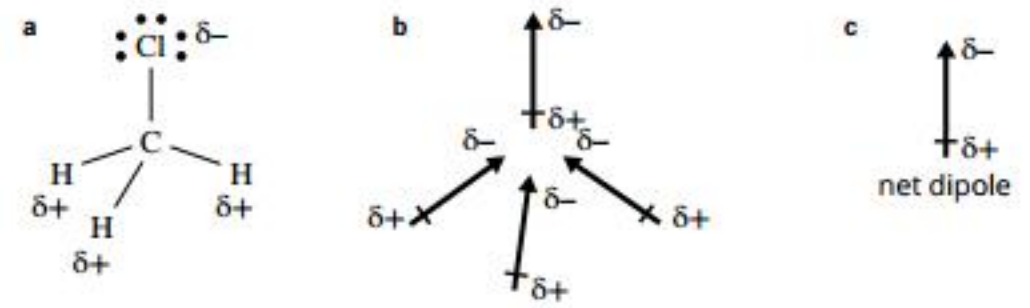


FIGURE 11.2.6 (a) Structure of a chloromethane molecule showing the partial charges on the atoms. (b) The individual dipoles are added together. (c) The result is a net dipole.

The ammonia molecule shown in Figure 11.2.7a is another example of an asymmetrical molecule. In this case, although all the bonds are identical their arrangement around the central nitrogen atom does not cancel out in all directions. The nitrogen atom is more electronegative than the hydrogen atom. Therefore, the nitrogen atom attracts electrons from the hydrogen atoms. The individual dipoles of the covalent bonds are shown in Figure 11.2.7b. These add to give the molecule a net dipole as shown in Figure 11.2.7c.

i In general, symmetrical molecules with polar bonds are overall non-polar and have no net dipole. In general, asymmetrical molecules with polar bonds are overall polar and have a net dipole.

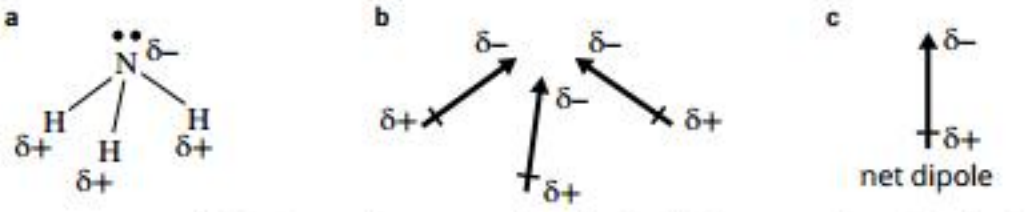
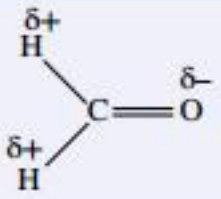
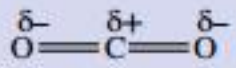
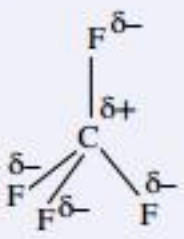
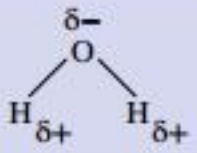
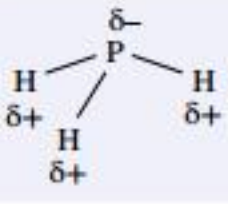


FIGURE 11.2.7 (a) Structure of an ammonia molecule. (b) An ammonia molecule showing the partial charges on the atoms. (c) The individual dipoles are added together. The result is a net dipole.

Table 11.2.1 shows more examples of how symmetry determines the polarity of covalent molecules.

TABLE 11.2.1 Examples of polar and non-polar covalent molecules

Molecule	Valence structure	Symmetrical/asymmetrical	Polar/non-polar
formaldehyde (methanal)		asymmetrical	polar
carbon dioxide		symmetrical	non-polar
tetrafluoromethane		symmetrical	non-polar
water		asymmetrical	polar
phosphine		asymmetrical	polar

11.2 Review

SUMMARY

- Electronegativity is the tendency of an atom in a covalent bond to attract electrons.
- The polarity of a covalent bond is the result of the difference in the electronegativities of the bonded atoms.
- As the electronegativity difference between two atoms increases, a covalent bond increases in polarity.
- Diatomic molecules containing the same type of atom are non-polar.
- The polarity of a polyatomic molecule depends upon the shape of the molecule and the individual bond dipoles.
- In general, symmetrical molecules with polar bonds are non-polar and asymmetrical molecules with polar bonds are polar.

KEY QUESTIONS

Describe

1 Define each of the following.
- **a** non-polar bond
- **b** polar bond

2 Use the electronegativity values given in Figure 11.2.1 on page 273 to list the following diatomic molecules in order of increasing polarity: HCl, N_2, HF, CO.

3 Identify which atom in H_2S has a partial negative charge. In your answer, provide the electronegativity values of the atoms.

4 Polarity (dipoles) in covalent bonds and molecules develops due to electronegativity differences of atoms.
- **a** Recall the definition of electronegativity.
- **b** State electronegativity trends of the periodic table.

Apply

5 Determine whether each of the following molecules is polar or non-polar.
- **a** CCl_4
- **b** $CHCl_3$
- **c** CH_2Cl_2
- **d** CH_3Cl
- **e** CH_4

6 For each of the following pairs of molecules, determine which is the polar molecule. On the polar molecule, indicate the polarities of the bonds and the direction of the net dipole.
- **a** CHF_3 or CF_4
- **b** NH_3 or CH_4

7 Consider the molecules NH_3 and H_2O. Determine which is the most polar.

Analyse

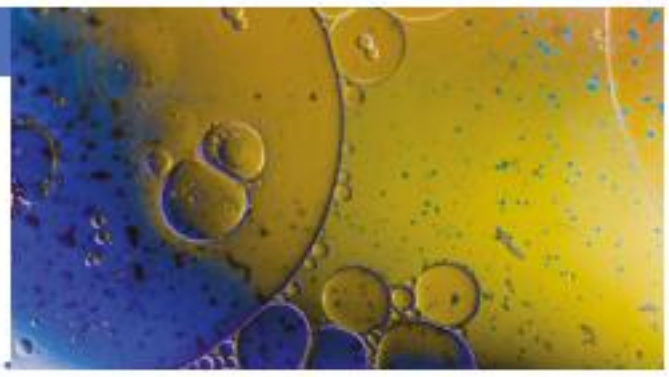
8 Describe how a molecule can have polar bonds but have no net dipole (be non-polar).

9 Determine the shape and polarity of phosphine, PH_3. Include a diagram of the molecule that shows bonding pairs and lone pairs.

11.3 Intermolecular forces

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the three types of intermolecular forces: dipole–dipole forces, hydrogen bonding and dispersion forces
- identify the types of intermolecular forces present between specific molecules in the liquid and solid states
- compare the strengths of the three types of intermolecular forces.



The molecules in covalent molecular substances are held together in the liquid and solid states by intermolecular forces. Intermolecular forces are the electrostatic attractive forces that exist *between* molecules and their effects are seen everywhere. If you have ever struggled to flatten out a sheet of cling wrap, then you have experienced the effects of intermolecular forces. Glue is an example of how intermolecular forces can be used to stick things together. The bubbles shown in Figure 11.3.1 are held together by intermolecular forces. Intermolecular forces are also responsible for creating the **surface tension** that allows insects to walk on water, as shown in Figure 11.3.2.

FIGURE 11.3.1 These bubbles are held together by intermolecular forces.

Intermolecular forces are 10–100 times weaker than strong intramolecular bonds such as ionic, metallic and covalent bonds. For example, as shown in Figure 11.3.3, diamond is a **covalent network solid** made up of a huge lattice of carbon atoms that are bonded with strong covalent bonds. This extremely strong lattice is the reason why diamond has a very high melting point and is the hardest natural substance on Earth.

The atoms in covalent molecules such as water (H_2O) and carbon dioxide (CO_2) are also held together by strong covalent bonds. However, covalent molecular substances tend to have much lower melting and boiling points than ionic, metallic and covalent network substances. This is because the forces between the molecules are much weaker, and it is these weak intermolecular attractions that are weakened when a covalent molecular substance is heated and converted from a solid to a liquid or from a liquid to a gas. Figure 11.3.4 shows the strong covalent bonds that hold the hydrogen and oxygen atoms together in a water molecule and the much weaker intermolecular forces that exist between the water molecules.

FIGURE 11.3.2 The surface tension created by intermolecular forces allows insects to walk on water.

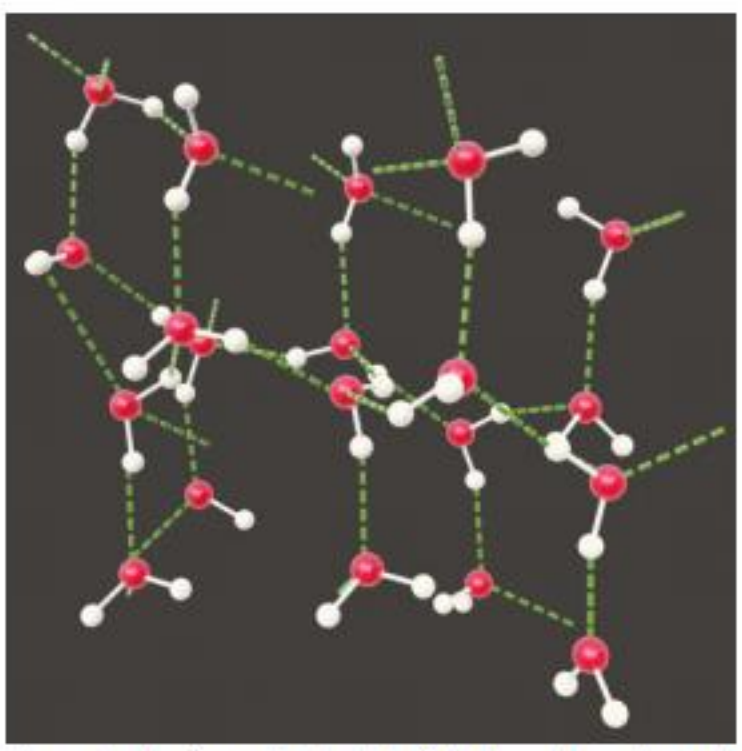


FIGURE 11.3.4 The intermolecular forces (dashed lines) between the water molecules are much weaker than the strong covalent bonds (solid lines) that hold the hydrogen and oxygen atoms together within the molecules.

FIGURE 11.3.3 Diamond is a covalent network solid made up of a lattice of carbon atoms that are bonded with strong covalent bonds.

TYPES OF INTERMOLECULAR FORCES

Many factors determine the type and strength of intermolecular forces present in covalent molecular substances, including the size, shape and polarity of the molecules.

There are three main types of intermolecular forces:

- dipole–dipole forces
- hydrogen bonding
- dispersion forces.

In this module, you will examine the nature of these types of intermolecular forces and begin to understand their role in determining the physical properties of covalent molecular substances.

Dipole–dipole forces

Dipole–dipole forces only occur between polar molecules. These forces result from the attraction between the positive and negative ends of polar molecules, as shown in Figure 11.3.5.

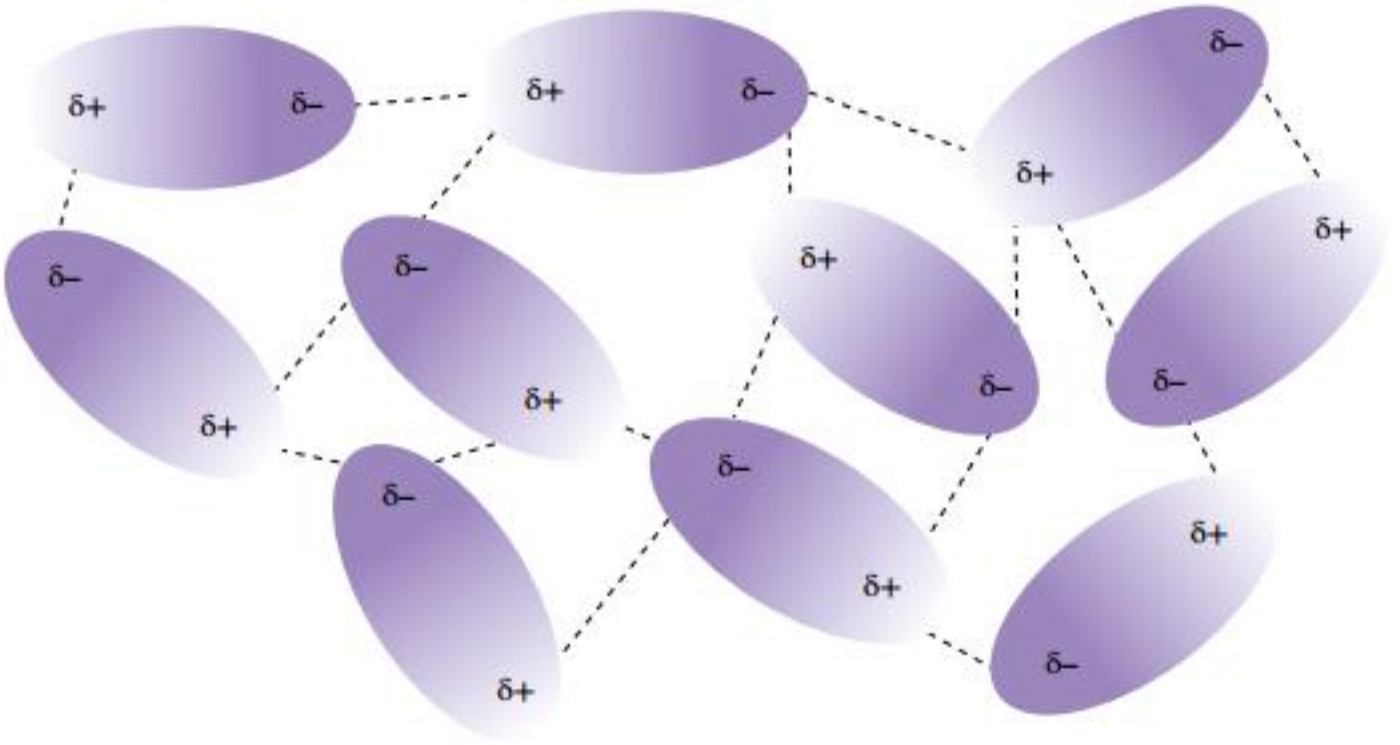


FIGURE 11.3.5 The positive and negative ends of polar molecules attract each other. Each molecule exists as a dipole.

Dipole–dipole forces are relatively weak since the partial charges (the δ+ and δ–) on the molecules are small. However, the more polar a molecule is, the stronger the dipole–dipole forces. The polarity will be larger when there is a large difference in the electronegativities of the atoms and a high degree of asymmetry in the shape of the molecule.

Dipole–dipole forces in a molecular substance directly affect its melting and boiling points. Substances that contain stronger dipole–dipole forces have higher melting and boiling points than substances of a similar size that contain either weaker dipole–dipole forces or no dipole–dipole forces at all. This is because it takes more energy (i.e. higher temperatures) to weaken the stronger dipole–dipole forces when the substance changes from a solid to a liquid or a liquid to a gas.

For example, compare methanal (also called formaldehyde, CH_2O) and ethane (CH_3CH_3), as shown in Figure 11.3.6. Methanal molecules are asymmetrical and polar. The molecules form dipole–dipole forces in the liquid state, which is the reason why methanal has a relatively high boiling point of –19°C. On the other hand, ethane molecules are symmetrical and non-polar. They do not form dipole–dipole forces resulting in ethane having a much lower boiling point of –88.5°C.

Molecules are more polar when there is a large difference in the electronegativities of the atoms and a high degree of asymmetry in the shape of the molecules. Molecules that are more polar form stronger dipole–dipole forces.

methanal, b.p. –19°C (polar) ethane, b.p. –88.5°C (non-polar)

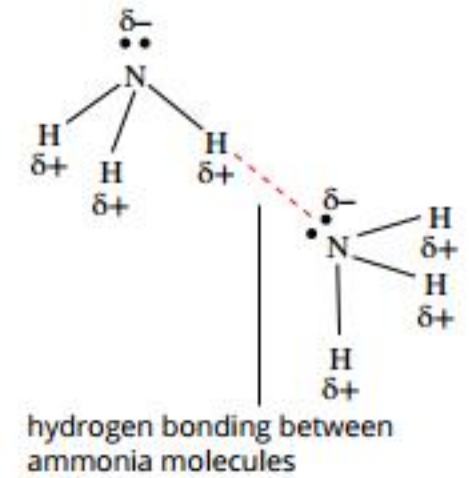
FIGURE 11.3.6 Molecular structures of methanal and ethane. Dipole–dipole forces exist between molecules of methanal because methanal is polar.

Hydrogen bonding

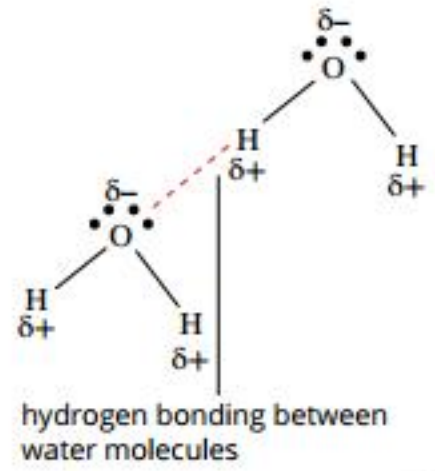
Hydrogen bonding is a particularly strong form of dipole–dipole force. Hydrogen bonding occurs between highly polar molecules in which a hydrogen atom is covalently bonded to an oxygen, a nitrogen or a fluorine atom.

Oxygen, nitrogen and fluorine atoms are small and highly electronegative. Therefore, when bonded with a hydrogen atom, they strongly attract the electron pair in the covalent bond and a large dipole results. Remember that hydrogen only has one electron and it is pulled towards the highly electronegative atom in the bond. The hydrogen nucleus (a proton) is therefore left exposed and is attracted to the lone pairs of electrons on the nitrogen, oxygen or fluorine atom of a neighbouring molecule. The small size of the hydrogen atom allows the neighbouring molecule to closely approach, and the resulting attractive force between molecules is relatively strong.

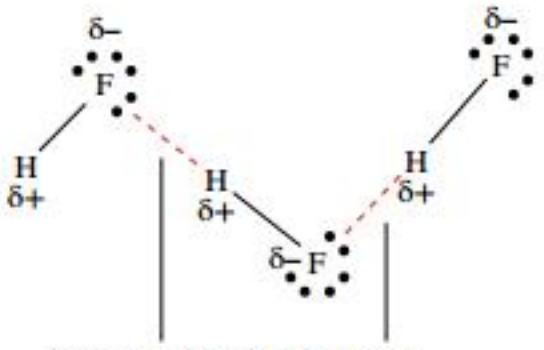
This intermolecular force is known as a hydrogen bond. It is approximately ten times stronger than other dipole–dipole forces but about one-tenth the strength of an ionic or a covalent bond. Figure 11.3.7 shows examples of hydrogen bonding among molecules that all contain a hydrogen atom covalently bonded to either an N, O or F atom.



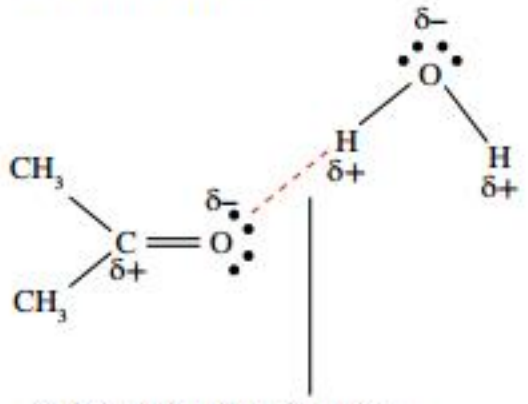
hydrogen bonding between ammonia molecules



hydrogen bonding between water molecules



hydrogen bonding between hydrogen fluoride molecules



hydrogen bonding between water and the oxygen atom of propanone (acetone)

FIGURE 11.3.7 Examples of hydrogen bonding between molecules containing a hydrogen atom covalently bonded to either an N, O or F atom.

The presence of hydrogen bonds results in much higher melting and boiling points. Figure 11.3.8 demonstrates the effect of hydrogen bonding on boiling point by comparing methanol to methanal and ethane. Recall that ethane contains non-polar molecules that do not form dipole–dipole forces. Methanal contains polar molecules that attract each other through dipole–dipole forces but not hydrogen bonds. Methanol, however, contains polar molecules that attract each other through hydrogen bonds. This is because each methanol molecule contains a hydrogen atom attached to an oxygen atom; as there is a large difference in electronegativities, this part of the methanol molecule is highly polar and can hydrogen bond with neighbouring methanol molecules. As a result, the boiling point of methanol (64.7°C) is significantly higher than the boiling points of methanal (–19°C) and ethane (–88.5°C).

ethane, b.p. –88.5°C (non-polar)

methanal, b.p. –19°C (polar)

methanol, b.p. 64.7°C (polar; hydrogen bonding between molecules)

FIGURE 11.3.8 Hydrogen bonding exists between molecules of methanol giving it a much higher boiling point than methanal and ethane.

There are two key requirements for hydrogen bonding:

1 a hydrogen atom covalently bonded to an oxygen, a nitrogen or a fluorine atom

2 a lone pair of electrons on the nitrogen, oxygen or fluorine atoms of neighbouring molecules.

Hydrogen bonding only occurs in highly polar molecules where a hydrogen atom is bonded to an oxygen, a nitrogen or a fluorine atom. It describes the attraction of a δ^+ H atom on one molecule with a δ^- F, N or O on another molecule.

You may wonder why other highly electronegative atoms do not form hydrogen bonds. For example, chlorine atoms have a high electronegativity but because they are larger atoms, the electron density is more spread out and less concentrated. This results in weaker dipole–dipole forces with the hydrogen atoms on neighbouring molecules.

Hydrogen bonding in water

Water is a very common substance with some unique properties, which are covered in more detail in Chapter 13. One such property is that ice floats because it is less dense than liquid water. By comparison, for most other substances the solid form is more dense than the liquid.

The fact that ice is less dense than liquid water can be explained by hydrogen bonding. Water has two hydrogen atoms attached to an oxygen atom in a bent shape. As shown in Figure 11.3.9, hydrogen bonds can form between the hydrogen atoms on one molecule and the lone pairs of electrons on the oxygen atoms of neighbouring molecules. In this way, a water molecule can form hydrogen bonds with four other water molecules.

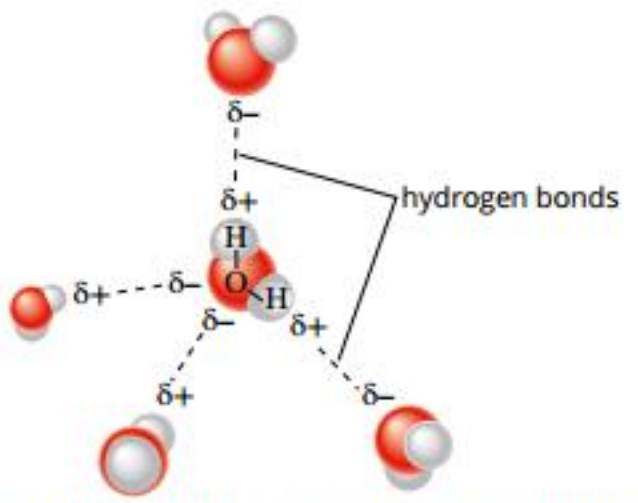


FIGURE 11.3.9 Each water molecule can form hydrogen bonds with four other water molecules.

The hydrogen bonding holds the water molecules in ice in a regular crystal lattice. In this lattice, the molecules are held further apart than in liquid water. As a result, ice is less dense and therefore floats in liquid water as shown in Figure 11.3.10 on page 283.

FIGURE 11.3.10 Ice floats because the water molecules form a crystal lattice in which they are spaced more widely apart than in liquid water. This arrangement means ice is less dense than liquid water.

When ice melts and forms liquid water, the density of the water increases rapidly. This is because the open crystal lattice collapses and the water molecules pack together more tightly.

However, as the temperature of the water increases further, water molecules in the liquid state move and vibrate more rapidly. The movement causes the molecules to spread further apart. As the molecules move further apart, the liquid becomes less dense.

Dispersion forces

Dipole–dipole forces (including hydrogen bonding) explain the intermolecular forces in polar substances. However, they do not explain the existence of intermolecular forces in non-polar substances.

We know that intermolecular forces are present in non-polar substances, otherwise they could not exist as liquids and solids. Without intermolecular forces, there would be nothing to hold the molecules together and non-polar substances would only exist as gases. However, there are many non-polar compounds that are liquids at room temperature (such as vegetable oil) and even non-polar solids (such as candle wax). In fact, all non-polar substances form liquids or solids if cooled to low enough temperatures. Even molecular hydrogen liquefies below –259°C.

The forces of attraction between non-polar molecules are known as **dispersion forces**. Dispersion forces are caused by **temporary dipoles** in the molecules that are the result of random movement of the electrons surrounding the molecules. These temporary dipoles are also known as **instantaneous dipoles**.

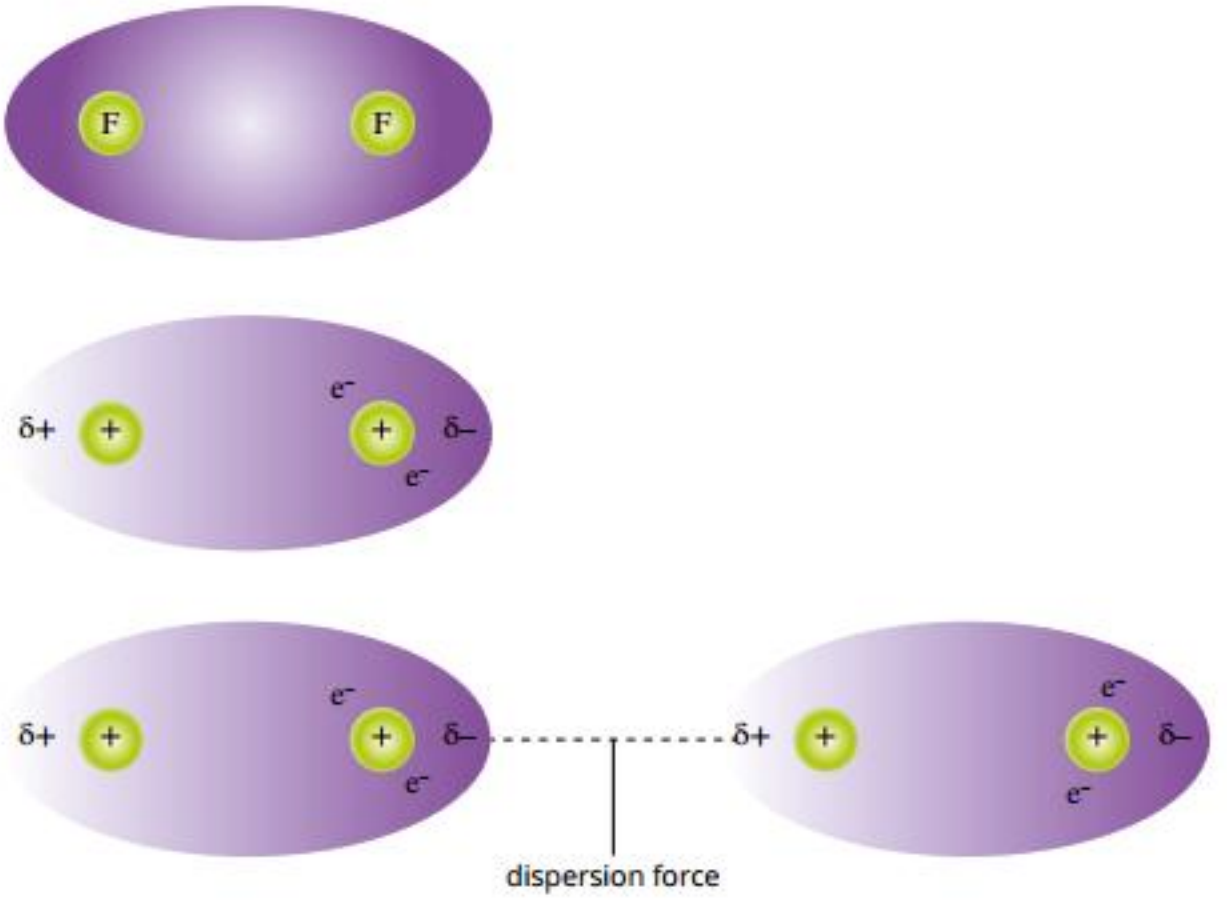
Dispersion forces are always present between molecules, no matter whether they are polar or non-polar, as electrons are constantly in motion within atoms. Consider the fluorine molecule in Figure 11.3.11a on page 284. F_2 is non-polar so the electrons are distributed evenly, as represented by the even shading in the figure.

However, this is only true over an average period of time. At any one time, the electrons may have a higher density at one end of the molecule and produce a temporary partial negative charge at that end, leaving a temporary partial positive charge on the opposite end, as shown in Figure 11.3.11b. The molecule is said to be **polarised** and the temporary electrical distortion is called a temporary dipole. These temporary dipoles can then induce (create) dipoles in neighbouring molecules, which subsequently induce dipoles in their neighbours and so on, as shown in Figures 11.3.11c and d.

a In a molecule, the electrons are constantly moving. In the case of a non-polar molecule, such as fluorine, the electrons spend an equal amount of time around each atom.

b Occasionally, the electrons gather more closely together at one end of the molecule, causing one end of the molecule to become partially negative and the other end to become partially positive. This is known as a temporary dipole.

c These temporary dipoles can then induce (create) dipoles in the neighbouring molecules.



d The neighbouring molecules then induce dipoles in their neighbours and so on. The temporary dipoles attract each other to create the intermolecular forces known as dispersion forces.

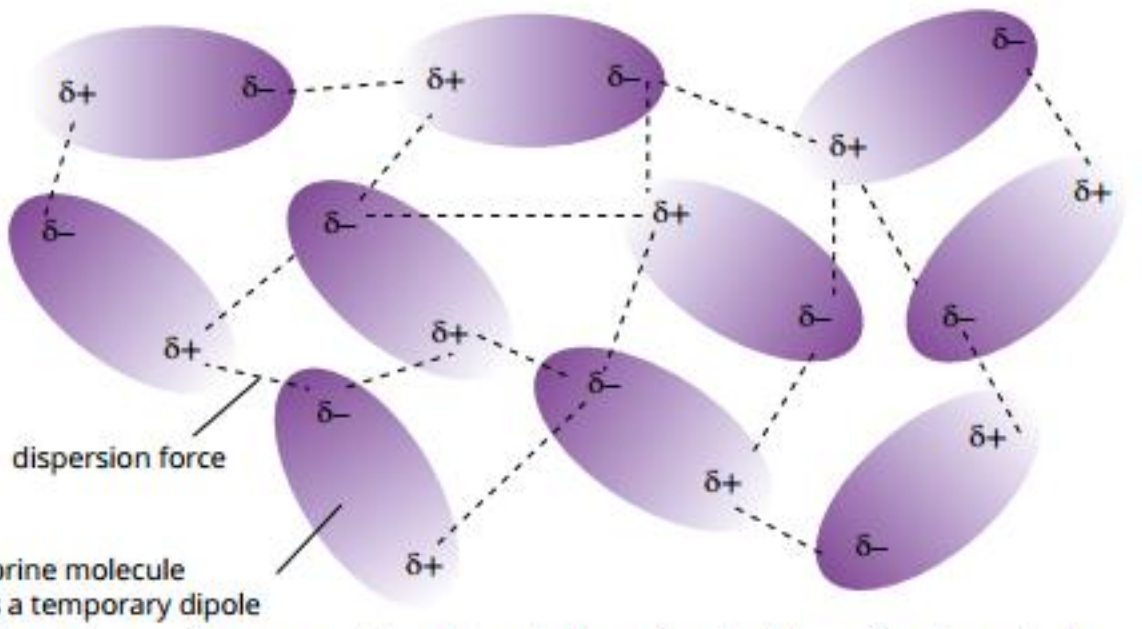


FIGURE 11.3.11 How dispersion forces form within non-polar substances. Diagrams a–d show dispersion forces forming between fluorine molecules.

Strength of dispersion forces

The strength of dispersion forces between molecules increases as the size of the molecules increase. This is because larger molecules contain more electrons that are, on average, further from the nuclei than those in smaller molecules. Because the electrons are further from the nuclei, they are less tightly held and more easily distorted. Larger molecules are therefore described as being more **polarisable** because they can form temporary dipoles more easily. As a result, larger molecules form stronger dispersion forces.

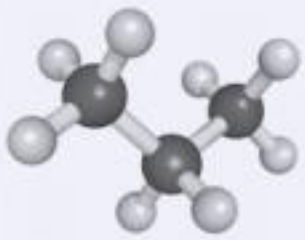
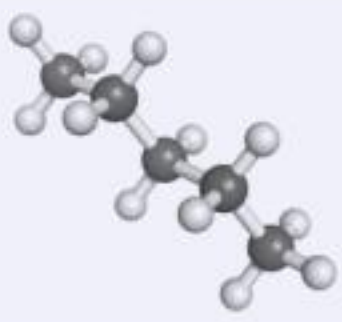
Table 11.3.1 shows the boiling points of the halogens (group 17 elements), which all form non-polar, diatomic molecules. The only forces between their molecules are dispersion forces. You can see that as molecular mass increases, the boiling point also increases. The comparison between increasing molecular mass and boiling point is a useful one. However, it is only used because, in general, as molecular mass increases, the size of the molecules and the number of electrons also increase. Consequently, the molecules become more polarisable and the dispersion forces become stronger, resulting in higher boiling points.

TABLE 11.3.1 The effect of dispersion forces on the boiling points of the halogens

Molecule	Molecular mass (amu)	Number of electrons	Boiling point (°C)
fluorine (F_2)	38.00	18	–188
chlorine (Cl_2)	70.90	34	–35
bromine (Br_2)	159.80	70	59
iodine (I_2)	253.80	106	184

An increase in molecule size due to increase in chain length results in change to strength of dispersion forces. Molecules that form long chains will tend to have stronger dispersion forces than molecules with smaller chains. For example, compare the boiling points of the alkanes propane, butane and pentane, which are shown in Table 11.3.2. As the carbon chain increases in size, the boiling point also increases. This is because the contact area over which the dispersion forces can act with neighbouring molecules increases; the dispersion forces become stronger and the boiling points of the substances increase.

TABLE 11.3.2 The effect of chain length on the boiling points of the alkanes propane, butane and pentane

Molecule	Molecular mass (amu)	Structure	Boiling point (°C)
propane (C_3H_8)	44.1		–42.2
butane (C_4H_{10})	58.1		–0.5
pentane (C_5H_{12})	72.1		36.3

Finally, the shape of a molecule affects the strength of the dispersion forces. Molecules that form long chains will tend to have stronger dispersion forces than more compact molecules with similar numbers of electrons.

For example, butane and methylpropane (Figure 11.3.12) have the same molecular mass and the same number of electrons because they both contain four carbon atoms and ten hydrogen atoms. The boiling point of butane is –0.5°C, while the boiling point of methylpropane is –11°C. The higher boiling point of butane is because of the different shapes of the two molecules; butane is a long molecule, while methylpropane is compact. Being less compact (more long and straight) means butane has more contact area to interact with its neighbouring molecules and form stronger dispersion forces.

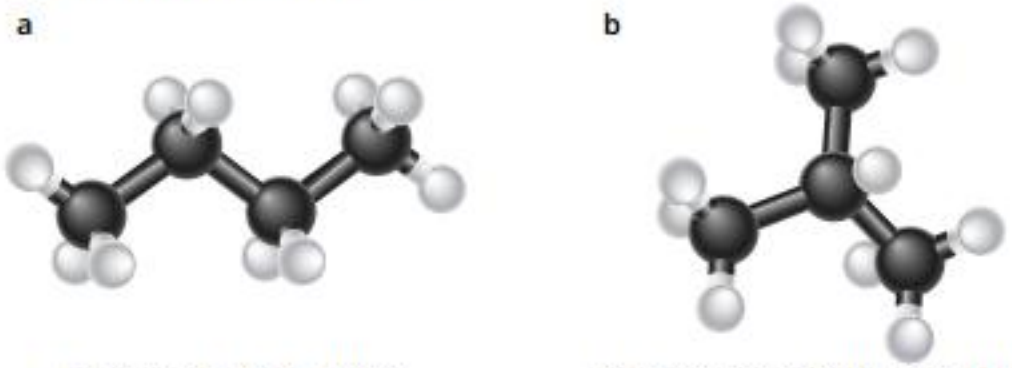


FIGURE 11.3.12 Butane has a higher boiling point than methylpropane due to its different shapes. The long straight shape promotes more intermolecular interactions compared to the compact round shape.

Comparing the strengths of intermolecular forces

Dispersion forces occur between all molecules, polar or non-polar. When comparing molecules of similar molecular mass, dispersion forces are weaker than dipole–dipole forces and much weaker than hydrogen bonds. For example, ethane (non-polar) has the lowest boiling point due to only dispersion forces (–88.5°C), methanal (polar) has a higher boiling point due to dipole–dipole forces and dispersion forces (–19°C), and methanol (with hydrogen bonds and dispersion forces) has the highest boiling point (64.7°C). This means that methanal and methanol have two types of intermolecular force existing between their molecules—a primary stronger one and the secondary weaker dispersion forces.

When comparing molecules of very different molecular masses, the dispersion forces in the heavier molecules can dominate over the dipole–dipole forces. Table 11.3.3 shows the boiling points of three hydrogen halides: hydrogen chloride (HCl), hydrogen bromide (HBr) and hydrogen iodide (HI). Hydrogen chloride is the most polar molecule and therefore forms the strongest dipole–dipole forces. However, hydrogen iodide has the highest boiling point. This is because it has the largest molecular mass resulting in particularly strong dispersion forces, which outweigh the effects of the dipole–dipole forces in hydrogen chloride.

TABLE 11.3.3 Comparison of the boiling points of three polar molecules

Substance	Molecular mass	Number of electrons	Boiling point (°C)
hydrogen chloride (HCl)	36.46	18	–85.1
hydrogen bromide (HBr)	80.91	36	–66.8
hydrogen iodide (HI)	127.91	54	–35.4

The boiling point of hydrogen fluoride (19.5°C) is much higher than any of these other compounds. This is because the hydrogen bonding between hydrogen fluoride molecules is much stronger than both the dispersion forces and the dipole–dipole forces between the other molecules listed in Table 11.3.3.

When comparing molecular substances with similar molecular masses, the strength of the intermolecular forces is in the order of dispersion < dipole–dipole < hydrogen bonding.

When comparing molecular substances of very different molecular masses, the dispersion forces can often outweigh the dipole–dipole forces. However, hydrogen bonds are generally the strongest of the three intermolecular forces.

11.3 Review

SUMMARY

- There are three types of intermolecular forces: dipole–dipole forces, hydrogen bonds and dispersion forces.
- Dipole–dipole forces are only present between polar molecules and are the result of the attraction between the partially positive and partially negative ends of polar molecules.
- Hydrogen bonding is a special type of dipole–dipole bonding occurring between highly polar molecules in which hydrogen atoms are covalently bonded to an oxygen, a nitrogen or a fluorine atom.
- A hydrogen bond is formed between the hydrogen atom in one molecule and lone pairs of electrons in an oxygen, a nitrogen or a fluorine atom in another molecule.
- Hydrogen bonding is the reason why ice floats in liquid water as it forms a crystal lattice where the molecules are spaced further apart than in liquid water. The greater spacing of molecules makes ice less dense than liquid water and so it floats on water.
- Dispersion forces occur between polar and non-polar molecules.
- Dispersion forces are the result of attractions between temporary dipoles that form in molecules.
- Temporary dipoles are due to random fluctuations in the distribution of electrons in molecules.
- Dispersion forces are stronger between molecules with larger molecular masses because it is easier to create temporary dipoles in molecules with a larger number of electrons.
- In molecules of similar molecular masses, the strength of the intermolecular forces increases in the following order: dispersion forces < dipole–dipole forces < hydrogen bonding.
- In molecules of very different molecular masses, dispersion forces can often outweigh the effects of dipole–dipole forces.
- Hydrogen bonds are generally the strongest of the three types of intermolecular forces.

KEY QUESTIONS

Describe

1 Identify the types of intermolecular forces of attraction that exist between:
- **a** polar molecules
- **b** non-polar molecules

2 State the three intermolecular forces in order of increasing strength of force.

Apply

3 Use your knowledge of the polarity of molecules and the different types of intermolecular forces to identify which of the following substances would contain dipole–dipole forces: bromine (Br_2), hydrogen chloride (HCl), methane (CH_4), tetrachloromethane (CCl_4), chloromethane (CH_3Cl).

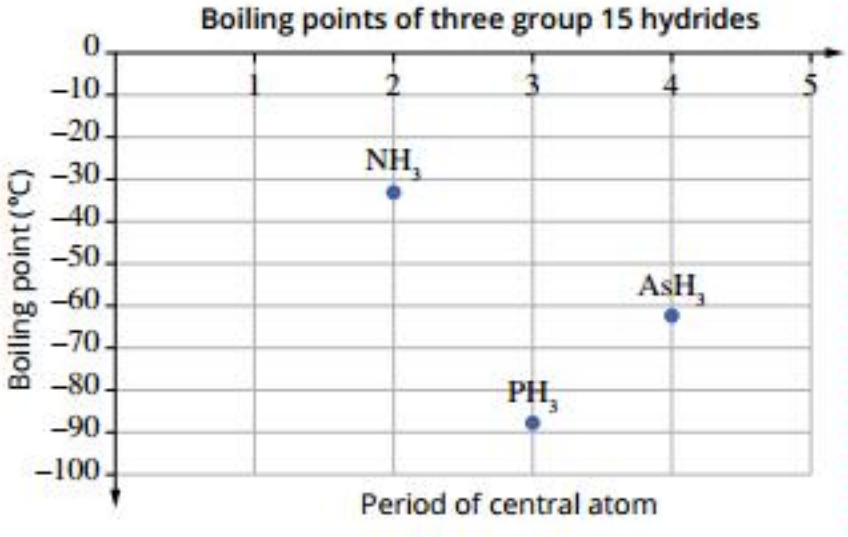
4 Use your knowledge of the features of a molecule required for hydrogen bonding to identify which of the following substances would contain hydrogen bonds: ammonia (NH_3), chloroform ($CHCl_3$), difluorine oxide (F_2O), hydrogen sulfide (H_2S), hydrogen (H_2)

5 Describe the factor(s) that cause an increase in intermolecular force for:
- **a** non-polar molecules
- **b** polar molecules

6 Identify which of the following observations can be explained by the presence of hydrogen bonding. For each provide a reason.
- **a** The boiling point of H_2O is higher than that of H_2S.
- **b** PH_3 has a lower boiling point than NH_3.
- **c** HBr has a lower boiling point than HCl.

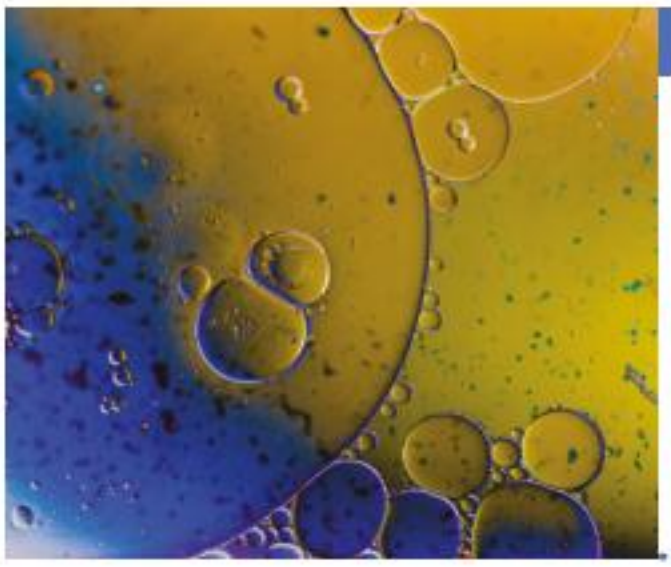
Analyse

7 The graph shows the boiling points of three group 15 hydrides.



- **a** For each hydride, identify the molecular shape, the intermolecular forces and the molar mass (low, medium or high).
- **b** Use this information to explain the observed differences in boiling points.

11.4 Properties of covalent molecular substances



BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe how intermolecular forces influence some of the properties of covalent molecular substances, such as vapour pressure, melting point, boiling point and solubility
- compare the vapour pressures of various covalent molecular substances and explain any differences
- compare the melting and boiling points of various covalent molecular substances and explain any differences
- describe the process of dissolving and explain why some covalent molecular substances are soluble or insoluble in particular solvents.

The physical properties of covalent molecular substances are primarily determined by the strength of the intermolecular forces within each substance. This module examines the relationship between the observable properties of covalent molecular substances and their intermolecular forces. Properties to be examined include vapour pressure, melting point, boiling point and solubility.

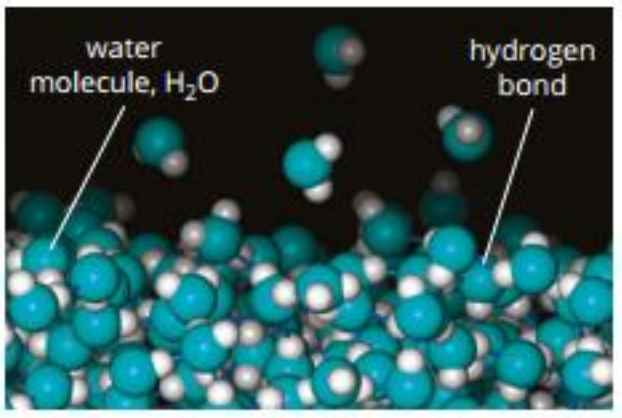


FIGURE 11.4.1 When water evaporates, the hydrogen bonds between the water molecules at the surface of the liquid are broken; however, the water molecules themselves remain intact (their structure does not change).

VAPOUR PRESSURE

When water is left in an open beaker it will completely evaporate. **Evaporation** occurs when the particles at the surface of the liquid are able to overcome the intermolecular forces of attraction within the liquid and escape. In the case of water, the H_2O molecules are kept together in the liquid state with hydrogen bonds. Some of the molecules at the surface of the liquid have enough energy to overcome these hydrogen bonds and move away from each other and from the surface—they evaporate. Given enough time, all of the water molecules will eventually escape from the surface of the liquid. Figure 11.4.1 shows this process. It is important to note that during evaporation the water molecules themselves remain intact; they move further away from each other as they transition from the **liquid state** to the **gaseous state**, but their structure does not change.

Now consider what will happen when water is put into a closed container. In this situation, not all of the water will evaporate. There is constant evaporation from the surface of the liquid but because the water particles that escape are moving around in the space above the liquid, some of them will hit the surface of the liquid and re-form hydrogen bonds—they condense. Eventually an **equilibrium** (or balance) will exist in which the rate of evaporation equals the rate of **condensation**; at this point the amount of liquid water and the amount of water vapour above the surface of the liquid will remain constant. This is depicted in Figure 11.4.2.

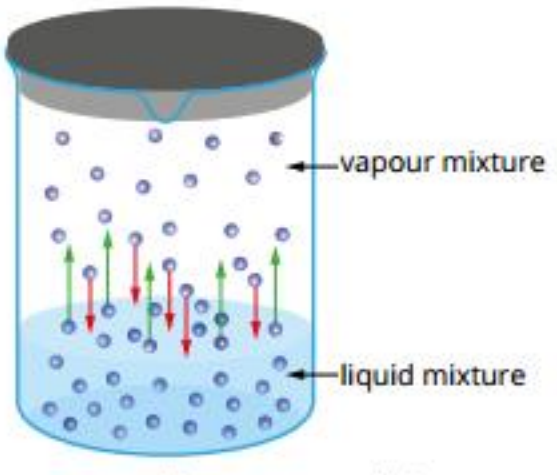


FIGURE 11.4.2 Vapour pressure is the pressure that the gaseous molecules exert on the closed container walls, where the rates of evaporation and condensation are equal.

The water vapour exerts a pressure on the container due to the collisions of the gaseous water molecules with the container wall. The pressure that a vapour exerts when in equilibrium with its liquid or solid state is known as the **vapour pressure**.

Liquids with stronger intermolecular forces have lower vapour pressures because the molecules are held together more tightly, making it harder for them to escape from the surface of the liquid. As a consequence, the rate at which molecules leave the surface of the liquid to form the vapour is much lower. Because there are fewer gas particles above the surface of the liquid, the vapour pressure is lower.

For example, water has a vapour pressure at room temperature of 3.17 kPa (kPa stands for **kilopascals**, one of many units used for pressure). On the other hand, butane, which is the liquid used as a lighter fluid, has a much higher vapour pressure of approximately 200 kPa. The difference in their vapour pressures can be explained by considering the intermolecular forces present in each of the liquids. As discussed above, water contains hydrogen bonds and, as you saw in Module 11.3, hydrogen bonds are the strongest of the intermolecular forces. Consequently, the water molecules are held together very tightly in the liquid and only a small proportion will be able to escape from the surface of the liquid to form water vapour. The vapour pressure of water is therefore relatively low. Butane (C_4H_{10}) is a non-polar substance so the only intermolecular forces holding the molecules together in the liquid are dispersion forces. These dispersion forces are much weaker than the hydrogen bonds in water and a greater proportion of butane molecules can escape the surface of the liquid to form a vapour. The vapour pressure of butane is therefore much higher than the vapour pressure of water.

i Covalent molecular substances with weaker intermolecular forces have higher vapour pressures as their molecules will readily dissociate and enter the gas state.

Worked example 11.4.1

COMPARING THE VAPOUR PRESSURES OF COVALENT MOLECULAR SUBSTANCES

Predict which would have the highest vapour pressure: carbon disulfide (CS_2) or ethanol (C_2H_5OH).	
Thinking	**Working**
Determine the intermolecular forces present in each of the substances.	Carbon disulfide is non-polar and only contains dispersion forces. Ethanol is polar and contains hydrogen bonds (due to the presence in each molecule of an oxygen atom attached to a hydrogen atom).
Determine which substance contains the strongest intermolecular forces.	Ethanol contains the strongest intermolecular forces (hydrogen bonds are stronger than dispersion forces).
Determine which substance will have the highest vapour pressure (this will be the substance with the weakest intermolecular forces).	Carbon disulfide will have the highest vapour pressure as it contains the weakest intermolecular forces.

➤ Try yourself 11.4.1

COMPARING THE VAPOUR PRESSURES OF COVALENT MOLECULAR SUBSTANCES

Predict which would have the highest vapour pressure: bromine (Br_2) or carbon disulfide (CS_2).

Vapour pressure and temperature

When a liquid is heated, it shows a greater tendency to evaporate. This is because its molecules have an increased kinetic energy, which allows them to more easily overcome the intermolecular forces holding them together. Therefore, as the temperature increases, the vapour pressure of the liquid also increases as more and more particles escape the surface of the liquid, transitioning to the gaseous state. Figure 11.4.3 shows the vapour pressures of four different liquids increasing with temperature. When a liquid's vapour pressure becomes equal to the atmospheric pressure of the surroundings, boiling occurs. At this point, bubbles of vapour are observed forming throughout the liquid. At sea level, atmospheric pressure is 101.325 kPa (or 1 atm). At this pressure, the boiling point is known as the normal boiling point.

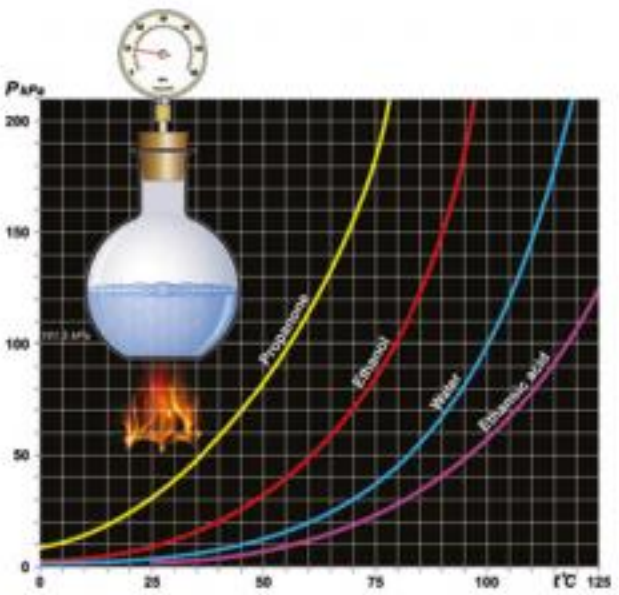


FIGURE 11.4.3 As temperature increases, the vapour pressure also increases. The boiling points of liquids can be determined by identifying the temperature at which the vapour pressure is equal to the atmospheric pressure. Here, at an atmospheric pressure of 101.325 kPa, ethanol has a boiling point of about 80°C and water about 100°C.

The normal boiling points of the four liquids in Figure 11.4.3 can be determined by identifying the temperature at which the vapour pressure is equal to 101.325 kPa.

MELTING AND BOILING POINTS

Covalent network solids (such as diamond, shown in Figure 11.3.3, page 279) and ionic compounds (such as sodium chloride) have very high melting and boiling points, which range from several hundred degrees Celsius to several thousand degrees Celsius. This is because they contain strong intramolecular covalent or ionic bonds that are broken when these substances are melted or boiled. Breaking these intramolecular bonds requires large amounts of energy.

However, when covalent molecular substances are melted or boiled, only intermolecular forces are disrupted; the intramolecular covalent bonds holding the atoms together within each molecule remain intact. Intermolecular forces are much weaker than strong intramolecular bonds and covalent molecular substances have much lower melting and boiling points as a result. Figure 11.4.4 depicts what happens to water molecules as water changes state from a solid to a liquid and then to a gas. As you can see, it is the hydrogen bonds between the water molecules that are broken and not the covalent O–H bonds within the molecules.

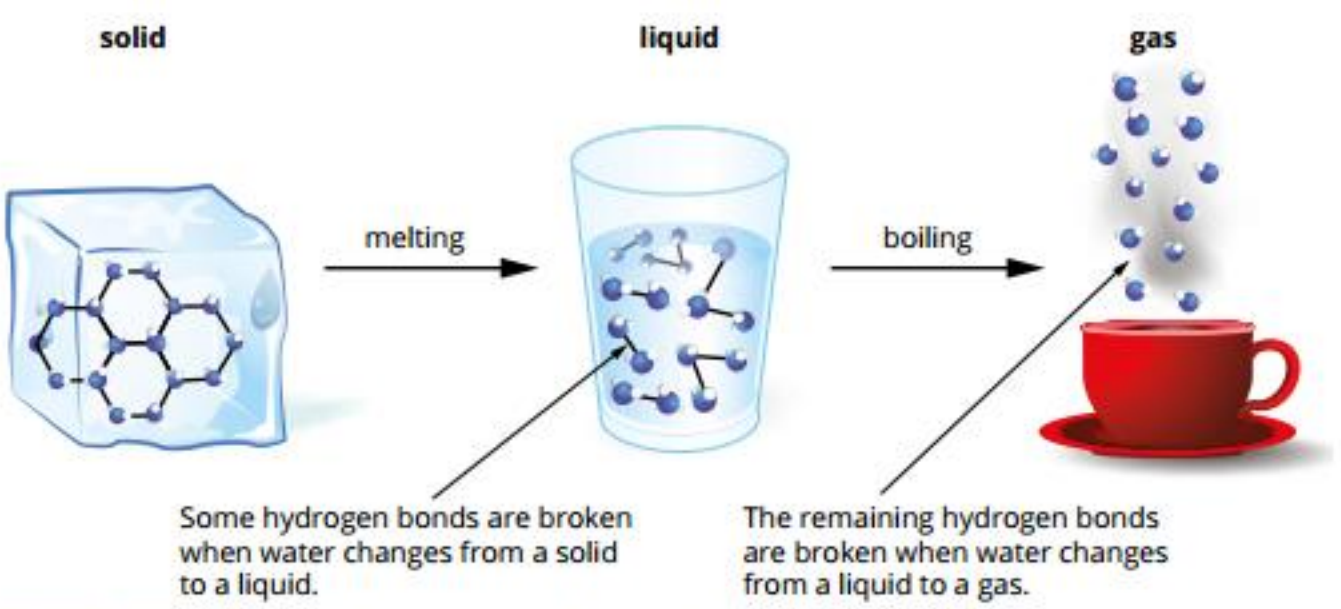

solid
liquid
gas
melting
boiling
Some hydrogen bonds are broken when water changes from a solid to a liquid.
The remaining hydrogen bonds are broken when water changes from a liquid to a gas.

FIGURE 11.4.4 When water changes from a solid to a liquid and then from a liquid to a gas, it is the hydrogen bonds between the water molecules that are broken and not the O–H covalent bonds within the molecules.

In Module 11.3, you looked at the different types of intermolecular forces and how their strengths affect the melting and boiling points of covalent molecular substances. In this part of Module 11.4, you will revise the main points from Module 11.3 and consolidate your understanding with specific examples.

In general, the strength of intermolecular forces increases as shown in Figure 11.4.5. Hydrogen bonding is the strongest intermolecular force, whereas dispersion forces are the weakest. The melting and boiling points of covalent molecular substances often depend on the different types of intermolecular forces present in each substance.

dispersion forces < dipole–dipole forces < hydrogen bonding

increasing strength of intermolecular forces

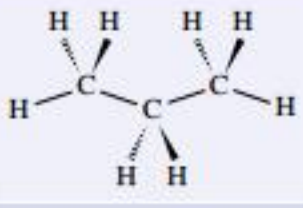
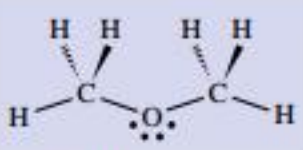
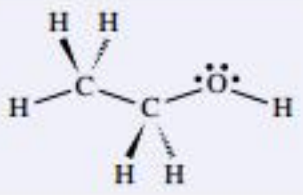
FIGURE 11.4.5 Increasing strength of the different types of intermolecular forces

However, you will recall that in the liquid and solid states, dispersion forces exist between all covalent molecular substances and that the strength of the dispersion forces tends to increase with an increase in molecular mass. Consequently, in substances that have large molecular masses, the contribution by the dispersion forces can be quite significant and often outweighs the dipole–dipole forces. The following examples illustrate the above points.

Comparing covalent molecular substances of similar molecular mass

Consider the following covalent molecular substances: propane ($CH_3CH_2CH_3$), methoxymethane (CH_3OCH_3) and ethanol (CH_3CH_2OH). They all have similar molecular masses, which means that, in general, the strength of their dispersion forces will also be similar. However, as a result of different intermolecular forces being present in each substance, the melting points for the three vary significantly, as do the boiling points. This is shown in Table 11.4.1. As you can see from the shapes of the molecules in Table 11.4.1, propane is non-polar, so the only intermolecular forces present in the substance are dispersion forces. Propane therefore has the lowest melting and boiling points. Methoxymethane is polar, which means that in addition to dispersion forces, the substance also contains dipole–dipole forces. These dipole–dipole forces are stronger than the dispersion forces and results in methoxymethane having higher melting and boiling points than propane. Ethanol molecules are polar and have a highly electronegative oxygen atom attached to a hydrogen atom, which means that the molecules can form hydrogen bonds. Because hydrogen bonding is the strongest intermolecular force, ethanol has the highest melting and boiling points of the three substances.

TABLE 11.4.1 Comparison of the melting and boiling points of covalent molecular substances with similar molecular masses

Substance	Molecular shape	Polarity	Relative molecular mass (amu)	Melting point (°C)	Boiling point (°C)
propane		non-polar	44.11	–188	–42
methoxymethane		polar	46.08	–142	–25
ethanol		polar	46.08	–117	78

Worked example 11.4.2

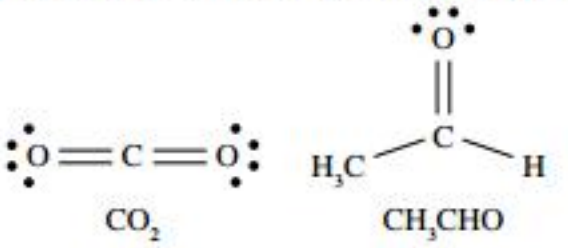
COMPARING THE MELTING AND BOILING POINTS OF MOLECULAR SUBSTANCES WITH SIMILAR MOLECULAR MASSES

Predict which would have the highest melting and boiling points: CH_4 or NH_3.	
Thinking	**Working**
Determine which intermolecular forces are present in each substance.	CH_4 is non-polar so only dispersion forces will be present. NH_3 is polar and can form hydrogen bonds because it contains a highly electronegative nitrogen atom covalently bonded to a hydrogen atom.
Determine which type of intermolecular force is the strongest.	Hydrogen bonding is generally stronger than dispersion forces.
Determine which substance has the highest melting and boiling point based on the intermolecular forces present.	NH_3 will have the highest melting and boiling point because of its stronger intermolecular forces.

➤ Try yourself 11.4.2

COMPARING THE MELTING AND BOILING POINTS OF MOLECULAR SUBSTANCES WITH SIMILAR MOLECULAR MASSES

Predict which would have the highest melting and boiling points: CO_2 or CH_3CHO.



Comparing covalent molecular substances that have very different molecular masses

Table 11.4.2 shows the melting and boiling points of some of the group 16 hydrides. Ignoring water for the moment and just focusing on the remaining hydrides, you can see that as the molecular mass increases, the melting and boiling points also increase (even though the polarities of the molecules, and consequently the dipole–dipole forces, decrease). This is due to the dispersion forces becoming stronger and being the dominant force between the heavier molecules.

Water (H_2O) has the smallest molecular mass of the group 16 hydrides and therefore the weakest dispersion forces. However, it melts at 0°C and boils at 100°C, which is considerably higher than the melting and boiling points of any of the other group 16 hydrides. This marked deviation from the general trend is attributed to the hydrogen bonding that exists between water molecules in the solid and liquid states. Hydrogen bonding is the strongest intermolecular force and can often outweigh very large dispersion forces; it is the reason why many substances containing hydrogen bonds between their molecules have particularly high melting and boiling points.

Hydrogen bonding is the strongest intermolecular force and can often outweigh even large dispersion forces.

TABLE 11.4.2 Comparison of the melting and boiling points of some of the group 16 hydrides

Hydride	Molecular mass (amu)	Melting point (°C)	Boiling point (°C)
H_2O	18.02	0	100
H_2S	34.08	–82	–60.7
H_2Se	80.99	–66	–41.5
H_2Te	129.62	–49	–2.2

Worked example 11.4.3

COMPARING THE MELTING AND BOILING POINTS OF MOLECULAR SUBSTANCES WITH VERY DIFFERENT MOLECULAR MASSES

Predict which would have the highest melting and boiling points: CH_4 or CF_4.

Thinking	Working
Compare the molecular masses of the molecules.	CF_4 is a much heavier molecule than CH_4.
Determine the intermolecular forces present in each substance.	Both are non-polar so dispersion forces are the only intermolecular forces present.
Determine which substance has the highest melting and boiling point based on the strength of the intermolecular forces.	The dispersion forces will be stronger in CF_4 than CH_4 because CF_4 has the largest molecular mass (and is therefore the larger molecule with more electrons; this makes it more polarisable). CF_4 has the highest melting and boiling points.

➤ Try yourself 11.4.3

COMPARING THE MELTING AND BOILING POINTS OF MOLECULAR SUBSTANCES WITH VERY DIFFERENT MOLECULAR MASSES

Predict which would have the highest melting and boiling points: O_2 or S_8.

Distillation

Each pure substance has a characteristic volatility and boiling point which can be explained by analysis of its intermolecular forces. **Distillation** is a useful technique which uses the physical property of boiling point to separate components of a liquid mixture (Figure 11.4.6). For example, a solution of ethanol (BP 78.5°C) and water (BP 100°C) can be separated via distillation. By slowly raising the liquid temperature to about 80°C, it is possible to heat and evaporate off the more volatile ethanol; the water is 'left behind' because it has a higher boiling point. Substance(s) that have entered the gaseous state are collected by cooling and condensation.

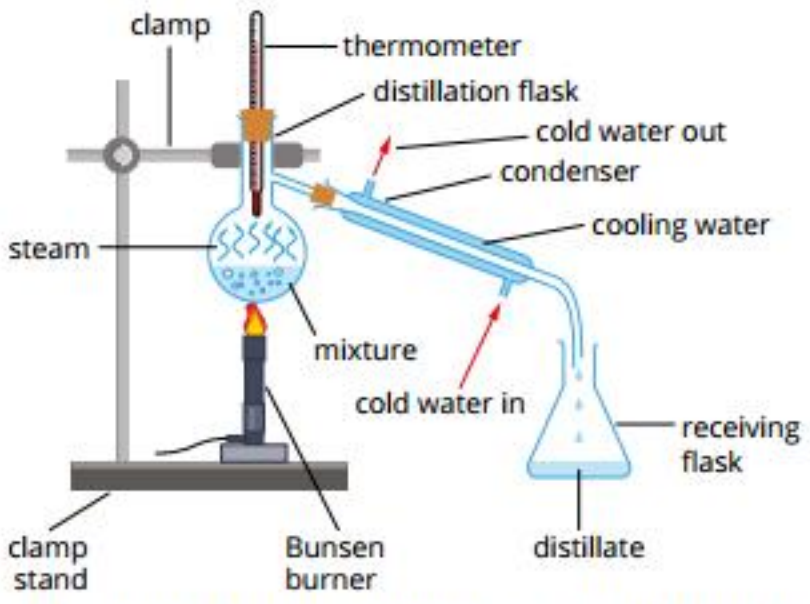


FIGURE 11.4.6 Typical distillation apparatus. A mixture is vaporised by heating the distillation flask. Gaseous vapours are condensed in the condenser tube, which is kept cool by a constant supply of water. The pure liquid solvent is collected in the receiving flask and compounds with higher boiling points remain in the distillation flask.

Distillation is used industrially on a very large scale as crude oil is separated into its components—a wide range of hydrocarbon molecules of different sizes. These compounds are non-polar hydrocarbons and have only dispersion forces between their molecules. This means that each will have a boiling point proportional to its molecule size. Known as **fractional distillation**, the technique separates the high molecular weight fuel and lubricating oils (containing about 10 to 20 carbon atoms) from moderately sized paraffin and petrol molecules (about 5 to 10 carbon atoms) to small LPG gas molecules (about 1 to 5 carbon atoms). The lower sized molecules (e.g. ethene) are feedstock for the plastics industry.

SOLUBILITY

The intermolecular forces present in a covalent molecular substance have a significant impact on its **solubility**. In general, a **solute** will dissolve in a **solvent** that has similar intermolecular forces. You can remember this with the saying 'like dissolves like'.

Pentane (C_5H_{12}), for example, readily dissolves in octane (C_8H_{18}). Both are non-polar liquids and only contain dispersion forces; they mix easily because of their similar intermolecular forces. During the dissolving process, energy is required to disrupt the dispersion forces in the pure liquids and separate the molecules. New dispersion forces then form between the pentane and octane molecules, as shown in Figure 11.4.7 on page 294. The energy that is required to disrupt the pentane–pentane and octane–octane dispersion forces in the pure liquids is compensated for by the energy that is released with the formation of the new pentane–octane dispersion forces.

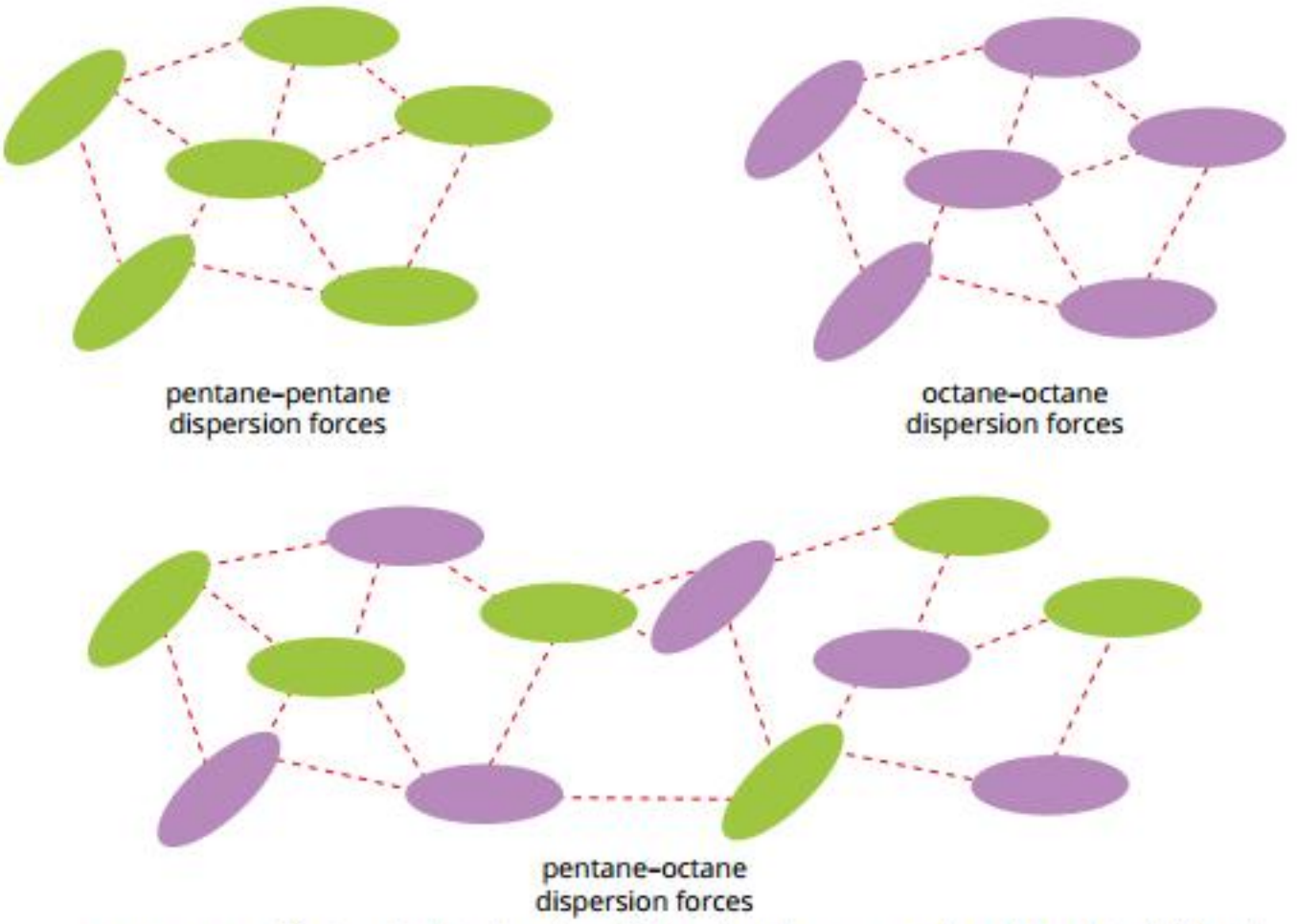


FIGURE 11.4.7 Pentane dissolves in octane. Both molecules are non-polar and are attracted to each other by dispersion forces.

While non-polar solutes dissolve in **non-polar solvents**, they will not easily dissolve in polar solvents such as water. This is because the intermolecular forces in the pure liquids are very different. For example, if pentane were to dissolve in water, because it is non-polar it could only form dispersion forces with the water molecules. The energy released on the formation of these dispersion forces would not be enough to compensate for the much larger amount of energy that would be required to break the hydrogen bonds between the water molecules in the first place. As a result, when pentane is added to water, two separate layers are visible with the pentane floating on top of the water; this is similar to what is observed when oil is added to water (oil is also non-polar and does not easily dissolve in water).

Lava lamps, such as the one shown in Figure 11.4.8, make use of the fact that non-polar substances are insoluble in water. They are made from a mixture of water and several different non-polar substances, such as oil and wax. When the lamps are turned on, the movement of the different layers throughout the mixture is very attractive.

Polar solutes dissolve in polar solvents because of their similar intermolecular forces. For example, methanol (CH_3OH) is very soluble in water because both substances contain hydrogen bonds. While the energy required to break the hydrogen bonds in the pure liquids is relatively large, the release of energy when new hydrogen bonds form between the methanol and water molecules compensates for this. Figure 11.4.9 shows the hydrogen bonds that form when methanol dissolves in water.

Solutes will generally only dissolve in solvents if their intermolecular forces are similar.

FIGURE 11.4.8 Lava lamps make use of the fact that non-polar substances do not dissolve in polar solvents like water.

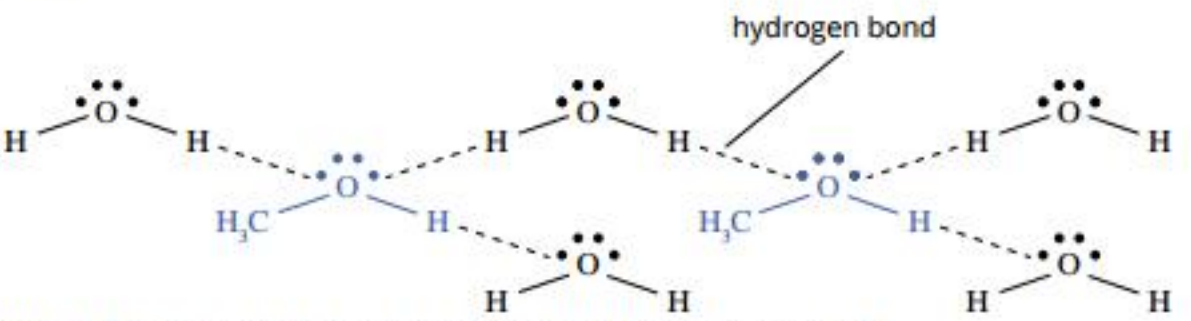


FIGURE 11.4.9 Hydrogen bonding between methanol and water molecules

Worked example 11.4.4

COMPARING THE SOLUBILITIES OF COVALENT MOLECULAR SUBSTANCES

Predict whether the following substances (the solutes) would be soluble in hexane (a non-polar solvent) or water.

a fluorine (F_2)

b difluoromethane (CH_2F_2)

Thinking	Working
Determine the intermolecular forces present in each of the solutes.	Fluorine is non-polar so only contains dispersion forces. Difluoromethane is polar and contains dipole–dipole bonds (due to the presence of electronegative chlorine atoms).
Determine the intermolecular forces present in each of the solvents.	Hexane is non-polar so only contains dispersion forces. Water is polar and contains hydrogen bonds.
A solute will dissolve in a solvent that has similar intermolecular forces. Therefore, pair up each solute with the solvent that closely matches its intermolecular forces.	Fluorine will be soluble in hexane, whereas difluoromethane will be soluble in water.

➤ Try yourself 11.4.4

COMPARING THE SOLUBILITIES OF COVALENT MOLECULAR SUBSTANCES

Predict which would have the highest solubility in hexane: iodine (I_2) or hydrogen iodide (HI).

VISCOSITY OF DIESEL

Sustainable and environmentally friendly fuels are becoming more common, and technologies for producing energy-rich fuels such as biodiesel are already in use. Chemists and engineers are working with agriculturalists to bring about efficiencies of scale that could allow the eventual switch from fossil fuel-sourced diesel (petrodiesel) to the analogous plant-based fuel (biodiesel). While the energy content of the two fuels is similar, there can be problems with using biodiesel in colder climates—its viscosity (resistance to flow) is significantly greater than that of petrodiesel. This lack of flow can affect transport, storage and use.

Higher **viscosity** is caused by stronger intermolecular forces. Figure 11.4.10 shows that biodiesel has greater polarity than petrodiesel due to the presence of the two O atoms. This means stronger intermolecular forces, causing a higher melting point, a higher boiling point and greater viscosity. Conversely, petrodiesel has weaker dispersion forces between its molecules, and as a result will have lower viscosity and better flow.

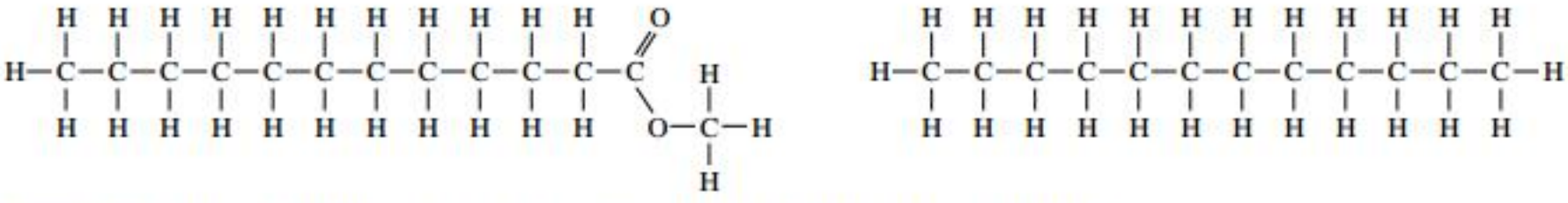


FIGURE 11.4.10 Chemical structure of the major constituents of biodiesel (left) and petrodiesel (right)

11.4 Review

SUMMARY

- Many of the physical properties of covalent molecular substances are determined by intermolecular forces. These properties include vapour pressure, melting point, boiling point and solubility.
- When covalent molecular substances change state, it is the intermolecular forces that are disrupted and not the intramolecular covalent bonds.
- Intermolecular forces are much weaker than strong intramolecular bonding such as ionic and covalent bonds.
- Vapour pressure is the pressure exerted by a gas above the surface of its liquid in a closed container.
- Liquids with stronger intermolecular forces have lower vapour pressures.
- A liquid's vapour pressure increases with temperature because the increased kinetic energy of the molecules enables them to overcome the intermolecular forces holding them together.
- Boiling occurs when a liquid's vapour pressure becomes equal to the atmospheric pressure of the surroundings.
- Melting and boiling points of covalent molecular substances are significantly lower than those of covalent network substances and ionic compounds.
- As the strength of the intermolecular forces increases, melting and boiling points also increase.
- Intermolecular forces present in a molecular substance have a significant impact on its solubility.
- Solutes will dissolve in solvents that have similar intermolecular forces.

KEY QUESTIONS

Describe

1 **a** Define the normal boiling point of a liquid.
b State the normal boiling point of water.

2 Identify what attractive forces are broken or disrupted when the following substances are melted or boiled.
a covalent molecular substances
b covalent network solids
c ionic substances

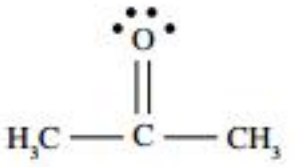
3 Indicate what is meant by the saying 'like dissolves like' when referring to a solute dissolving in a solvent.

Apply

4 The following statements refer to the vapour pressures of covalent molecular substances. Use your understanding of intermolecular forces to explain each statement.
a A liquid with strong intermolecular forces has a low vapour pressure.
b An increase in temperature leads to an increase in a liquid's vapour pressure.

5 **a** Describe the changes that occur at the molecular level when a covalent molecular liquid is heated to boiling point.
b Explain why covalent molecular substances have lower melting and boiling points than covalent network solids and ionic compounds.

6 Use your understanding of how intermolecular forces affect solubility to determine whether each of the following covalent molecular substances would be soluble in a polar solvent, such as water, or a non-polar solvent, such as hexane.
a methane (CH_4)
b ethanol (C_2H_5OH)
c bromine (Br_2)
d propanone (CH_3COCH_3) (the structure of propanone is shown below)



Analyse

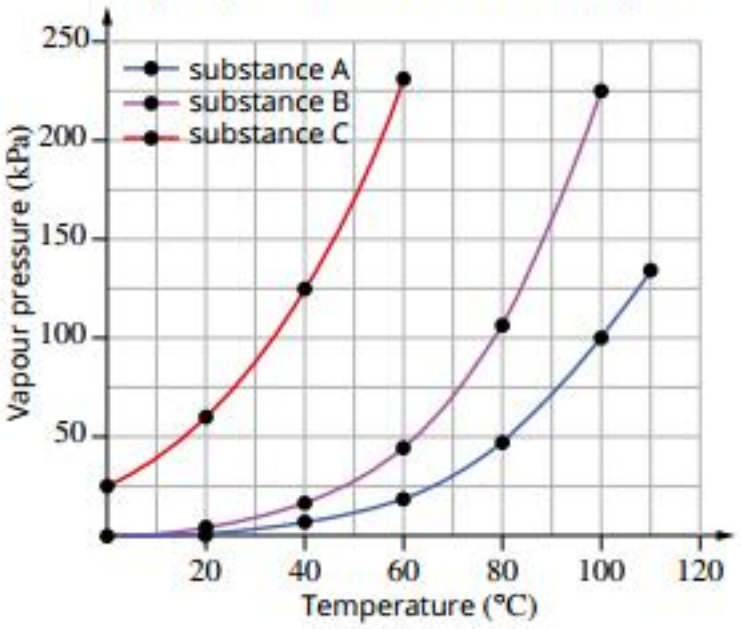
7 Pentane (C_5H_{12}) and octane (C_8H_{18}) are both non-polar and liquids at room temperature. Predict which will have the highest vapour pressure at this temperature and explain your answer.

8 For each pair of covalent molecular substances, analyse their structures and determine the reason for the differences in their boiling points.
a F_2, boiling point = −188°C; HCl, boiling point = −85°C
b PH_3, boiling point = −88°C; NH_3, boiling point = −33°C
c CH_4, boiling point = −161°C; CCl_4, boiling point = 77°C

9 Determine why pentane (C_5H_{12}) is soluble in carbon tetrachloride (CCl_4), whereas ethanol (C_2H_5OH) is insoluble in carbon tetrachloride.

10 The figure below shows the vapour pressure curves for three liquids that are covalent molecular substances. Use the graph to answer the questions that follow.

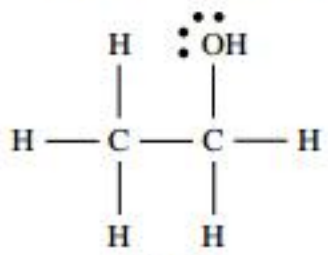
Vapour pressure curves for three liquids



a Conclude which substance (A, B or C) contains the strongest intermolecular forces.

b Conclude which substance (A, B or C) contains the weakest intermolecular forces.

c Knowing that the three substances are ethanol, water and diethyl ether (the structures of ethanol and diethyl ether are shown) and that water is substance A, determine the identities of substances B and C. Explain your answer.



ethanol

diethyl ether

d Deduce from their structures, why there is a difference in vapour pressures between substance A and substance B.

11 The boiling points of a series of organic alcohols are given in the table below and shown on the graph following. You will notice that as you move down the series, the chain length of the alcohols increases by one carbon each time.

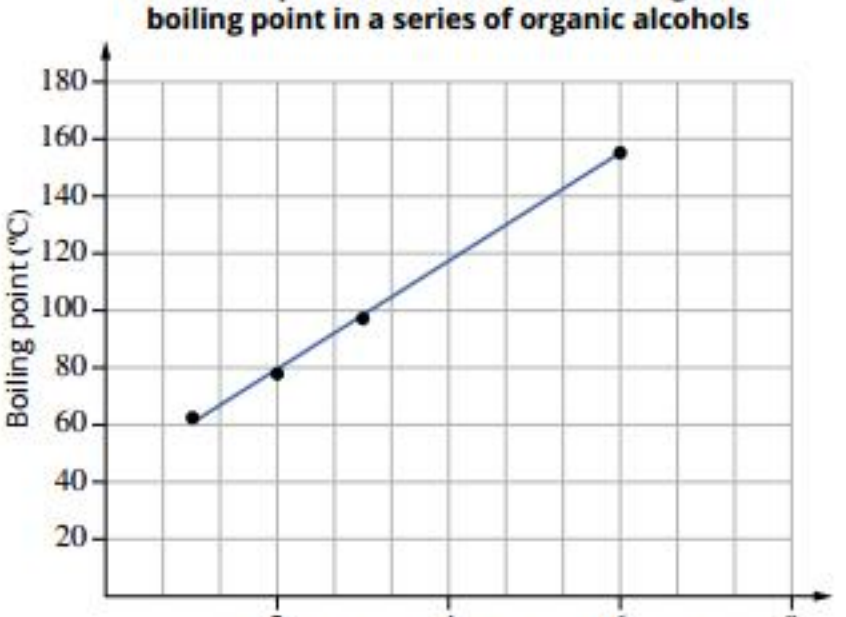
a Use the graph to predict the boiling point of the alcohols butan-1-ol and pentan-1-ol.

b Determine which type of intermolecular force is responsible for the increase in boiling points within this series of alcohols.

c Explain why the boiling points increase as the carbon chain length increases.

Alcohol	Carbon chain length	Boiling point (°C)
methanol (CH_3OH)	1	64.5
ethanol (CH_3CH_2OH)	2	78.5
propanol ($CH_3CH_2CH_2OH$)	3	97.2
butanol ($CH_3CH_2CH_2CH_2OH$)	4	?
petan-1-ol ($CH_3CH_2CH_2CH_2CH_2OH$)	5	?
hexan-1-ol ($CH_3CH_2CH_2CH_2CH_2CH_2OH$)	6	157

Relationship between carbon chain length and boiling point in a series of organic alcohols



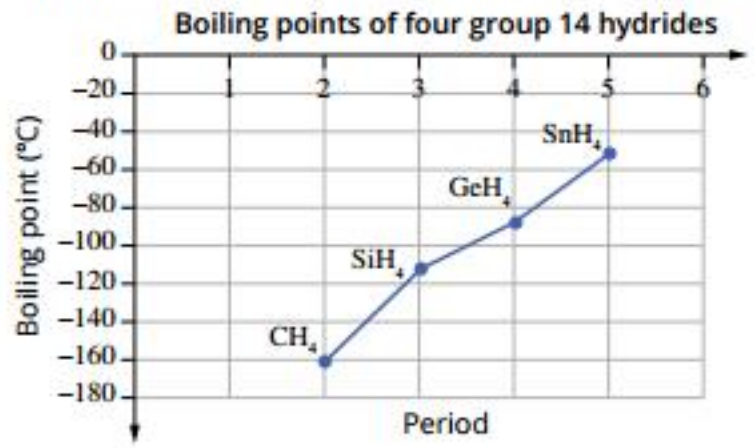
12 A covalent molecular substance is found to be very soluble in cyclohexane, a non-polar solvent, and only slightly soluble in water (polar). Deduce the type of intermolecular force(s) that exist in the substance.

13 'CF_4 has higher vapour pressure than H_2O'. Use your understanding of intermolecular forces to predict if this statement is correct and justify your response.

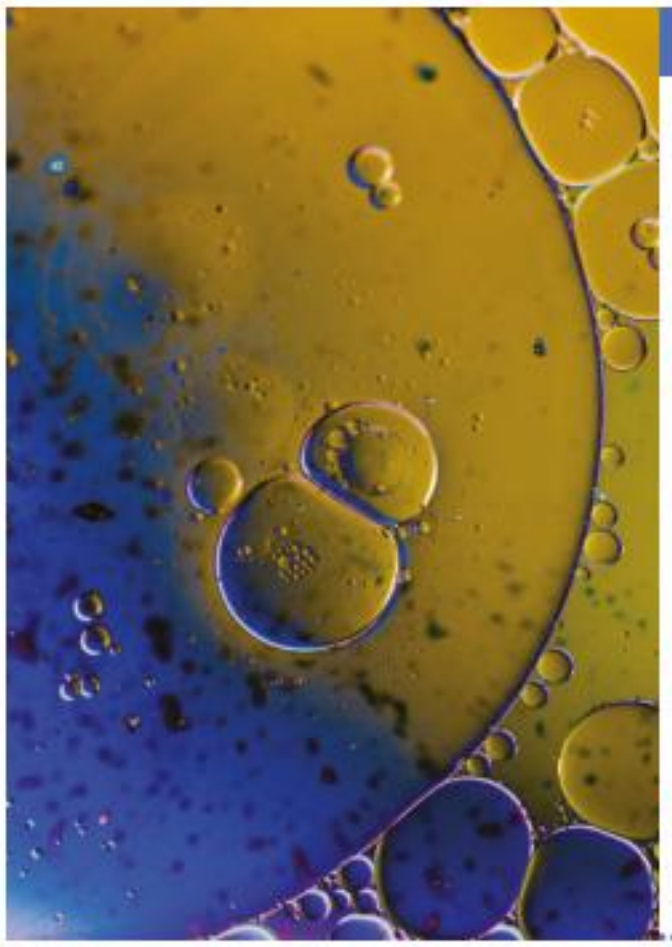
14 The boiling point of sulfur dioxide is −10°C whereas the boiling point of carbon dioxide is −57°C. Account for this difference.

15 Explain the boiling point trend for group 14 hydrides.

Boiling points of four group 14 hydrides



11.5 Chromatography



BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that different chromatography techniques use common principles that enable the separation and identification of the components in a mixture
- recognise simple forms of this technique such as paper chromatography and thin-layer chromatography
- understand that separation of components of a mixture is due to differences in affinity for the mobile and stationary phases and is due to intermolecular forces
- understand that components separate during chromatography because of how strongly they adsorb to the stationary phase and desorb back into the mobile phase
- understand that the polarities of the components and of the mobile and stationary phases determine the degree of separation of the components of the mixture.
- understand that in paper and thin-layer chromatography, the components in a mixture can be qualitatively identified by comparison with known standards and determination of R_f values.

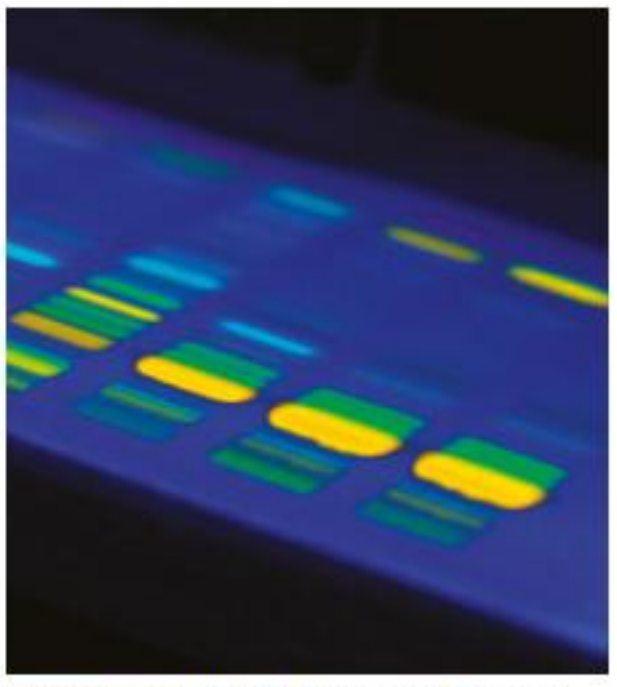


FIGURE 11.5.1 These glowing bands, viewed under fluorescent lighting, are individual chemical components that have been separated from a mixture by thin-layer chromatography. The individual components can then be identified using R_f values compared to standards or mass spectrometry.

In Module 11.4, you saw how the physical properties of covalent substances are dictated by the polarity of molecules and the intermolecular forces between molecules. In this module, we show how polarity and intermolecular forces can be used in the application of a separation technique called **chromatography**. Two simple forms of the technique, paper chromatography and thin-layer chromatography, use the same principles of separation. Chromatography separates components of a mixture and can be used for both **qualitative analysis** and **quantitative analysis** to identify numerous inorganic and organic substances in a chemical mixture. Contaminants in water, toxic gases in air, impurities in food and drugs present in blood can be detected and measured. A feature of chromatography is that it can be performed on very small samples and with solutions of low concentrations. When separated, the various components often appear as distinct bands or as a **chromatogram**, as seen in Figure 11.5.1.

In this module, you will learn about the underlying principles of **chromatography** and about two simple forms of the technique called **paper chromatography** and **thin-layer chromatography**. Then, you will see how these two-dimensional tests can be expanded to a three-dimensional structure in **column chromatography.** These basic techniques have been developed into the sophisticated and sensitive instruments that are used in medicine, forensics and industry.

HOW CHROMATOGRAPHY WORKS

You can perform a simple chromatography experiment by putting spots of ink from felt-tip pens near one end of a strip of filter paper. The filter paper can then be suspended so the end closest to the ink spots is just immersed in water.

The original position of the ink spots on the paper is called the **origin**. The inks are a mixture of different-coloured chemicals. As the water soaks up the paper, the components of the inks are carried upwards at different rates and separate into spots of different colours. When the paper is removed from the water, the positions of the individual components are analysed, as seen in Figure 11.5.2.

Each spot contains one of the components that are present in the ink mixture. The pattern of bands or spots is called a chromatogram. In the laboratory, paper chromatography is performed with high-quality absorbent paper, similar to filter paper.

All methods of chromatography have a:

- **stationary phase**
- moving or **mobile phase**.

In the simple experiment using inks and paper, the stationary phase is a thin layer of water adsorbed to the paper and the mobile phase is the water.

As the components in the ink are swept upwards over the stationary phase by the **solvent**, they undergo a continual process of **adsorption** (onto the stationary phase), followed by **desorption** and dissolving (into the mobile phase).

The amount that each component moves mainly depends on:

- how strongly the component adsorbs onto the stationary phase
- how readily the component dissolves in the mobile phase.

The components of the mixture separate because they undergo these two processes to a different degree.

When both **solute** and solvent contain molecules or ions with charge or partially charged areas, dissolving occurs (as described in Chapter 13). Water is a **polar solvent**. If water is used as the mobile phase, the more polar components will form dipole–dipole interactions and hydrogen bonds with the water molecules. These interactions result in the polar components, being highly soluble in a polar aqueous solvent, forming bonds with the mobile phase and dissolving in it. They will stay in the mobile phase and will tend to move further up the paper faster than the less polar or **non-polar** components.

Adsorbing onto the stationary phase and desorbing into the mobile phase are opposing processes that occur simultaneously. The processes can be likened to a 'tug of war' with the components in the mixture being pulled in two directions. The degree to which a component undergoes these processes is determined by its physical properties, such as size, polarity and charge, and so its rate of movement through the medium, using a given solvent and temperature, will be unique. To maximise chromatographic separation of compounds of interest, chemists can alter both the stationary phase medium and the mobile phase solvent. In our studies, we will describe the use of polar and non-polar solvents as mobile phases and the use of paper and thin-layer chromatography as stationary phases.

FIGURE 11.5.2 Paper chromatography can be used to separate mixtures of inks into their separate components.

The term 'adsorption' describes the adhesion of molecules or substances to the surface of a solid or liquid. This is why the stationary phase in chromatography is either a solid or a liquid on a solid support. The mobile phase is a liquid or gas state.

PAPER AND THIN-LAYER CHROMATOGRAPHY

In the laboratory, paper chromatography (Figure 11.5.2) is performed on high-quality absorbent paper, similar to filter paper, as the stationary phase. Being primarily cellulose, it has a polar surface with surface OH groups. Thin-layer chromatography (TLC) is very similar to paper chromatography. In this case, the stationary phase is a thin layer of a fine powder, also polar, such as alumina (aluminium oxide) or silica gel, spread on a glass or plastic plate. Both techniques are useful for qualitative analysis. They can indicate which chemicals are present in the mixture. Paper chromatography cannot indicate the specific concentration of any component. However, bands for specific components in thin-layer chromatography can be removed from the plate and the component isolated, allowing an approximate concentration to be calculated. More sophisticated methods, such as gas chromatography (GC) and high-performance liquid chromatography (HPLC), give more accurate and precise quantitative results.

In both paper and thin-layer chromatography, a small spot of the solution of the sample to be analysed is placed on one end of the chromatography paper or plate. The position of this spot is called the origin. The paper or plate is then placed in a container with solvent. The origin must be a little above the level of the solvent so that the components can be transported up the paper or plate and not dissolve into the liquid in the container.

'Solvent front' is the term used to describe the movement of the solvent during chromatography. It is visible as the wet moving edge of the solvent as it travels up the stationary phase.

As the solvent rises up the paper or plate, the components of each sample separate, as shown in Figure 11.5.3. The paper or plate is removed from the solvent before the liquid reaches the top, and the final position (distance from the origin) of each component and the **solvent front** are recorded. To improve the accuracy of the results and allow measurements to be made, the paper or plate is dried quickly to prevent the components and solvent continuing to rise beyond the end of the paper or plate.

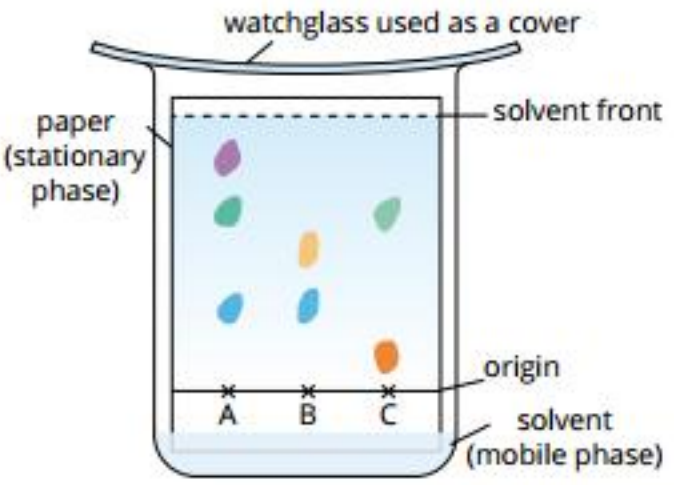


FIGURE 11.5.3 Paper chromatography of three different food colours (A, B and C) using water as solvent

Although the components of inks can be seen easily in the chromatogram in Figure 11.5.2, most compounds are colourless and must be made visible. Many organic compounds **fluoresce** and appear blue when viewed under ultraviolet light. Another way to make colourless components visible is to spray them with a chemical that reacts to form coloured or fluorescent compounds (Figure 11.5.1 on page 298).

The choice between paper and thin-layer chromatography depends upon the sample being analysed. Advantages of each method are given in Table 11.5.1.

TABLE 11.5.1 A comparison of paper and thin-layer chromatography

Paper chromatography	Thin-layer chromatography
is cheap	detects smaller amounts
requires little preparation	achieves better separation of less polar compounds
is more efficient for polar and water-soluble compounds	can use corrosive materials such as organic solvents
is easy to handle and store	has a wide range of stationary phases

Importance of the polarity of the stationary phase and the mobile phase

As you have seen, the actual process of separation depends largely on the polarity of the chemicals in both the stationary and mobile phases, as well as the polarity of each component. In order to improve the degree of separation of components, a less polar stationary phase could be combined with a polar mobile phase or vice versa.

In Figure 11.5.3 both the stationary and mobile phases are polar to different degrees. The orange part of the food colour C is almost non-polar (showing limited solubility in water), whereas the green component is quite polar and has moved up the paper with the mobile phase. These two components have been well separated and can be more easily identified, as you will see below.

Chromatography results—using R_f values and standards

The components in a mixture separated by chromatography can be identified in two ways:

1 by calculating the **retardation factor (R_f)** of the sample
2 by including **standards** of known chemicals on the same chromatogram as the unknown sample.

Method 1: Calculating R_f values

Each component of a mixture will travel a specific distance up the stationary phase. By comparing the distance travelled by the component from the origin to the total distance travelled by the solvent from the origin to the solvent front, you can calculate a ratio called the retardation factor.

i The retardation factor (R_f) for a component is given by:

$$R_f = \frac{\text{distance the component travels from the origin}}{\text{distance the solvent front travels from the origin}}$$

You can see from Figure 11.5.4 that:

- R_f values are always less than one
- the component most strongly adsorbed onto the stationary phase moves the shortest distance and has the lowest R_f value
- the component most soluble in the mobile phase moves the furthest and has the largest R_f value.

Each component has a characteristic R_f value for the conditions under which the chromatogram was obtained. By comparing the R_f values of components of a particular mixture with the R_f values of known substances determined under identical conditions, you can identify the components present in a mixture.

In this method, the distance moved by the solvent front is not critical. R_f values are a ratio and have no units. The proportion of the distance moved from the origin (the R_f value) stays the same provided the conditions under which the chromatogram is obtained are the same. This means the R_f values of unknown spots can be compared against a table of R_f values of common materials.

However, changes in the temperature, the type of stationary phase, the amount of water vapour (around the plate or paper) and the type of solvent all change the R_f value for a particular chemical. For the R_f value of a component to be comparable to a set of standard R_f values, they must be determined under identical conditions.

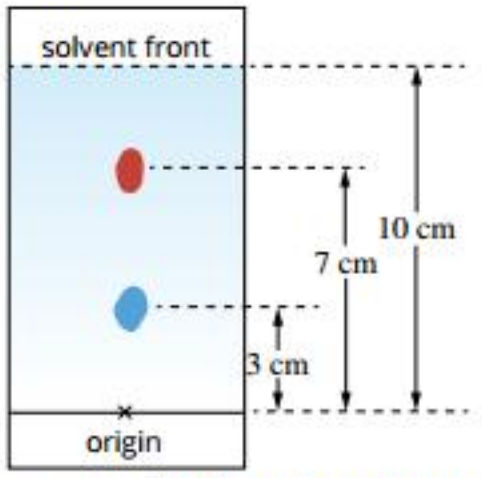


FIGURE 11.5.4 A thin-layer chromatogram of a sample with two components. The distances from the origin enable you to calculate R_f.

i For the R_f value of a component to be comparable to a set of standard R_f values, they must be determined under identical conditions.

Worked example 11.5.1

CALCULATING R_f VALUES

Using Figure 11.5.4, calculate the R_f value of the blue component.	
Thinking	**Working**
Record the distance the component has moved from the origin and the distance the solvent front has moved from the origin.	The distance the blue component has moved from the origin is 3 cm. The distance the solvent front has moved from the origin is 10 cm.
$R_f = \frac{\text{distance the component travels from the origin}}{\text{distance the solvent front travels from the origin}}$	$R_f(\text{blue component}) = \frac{3}{10} = 0.3$

➤ Try yourself 11.5.1

CALCULATING R_f VALUES

Using Figure 11.5.4, calculate the R_f value of the red component.

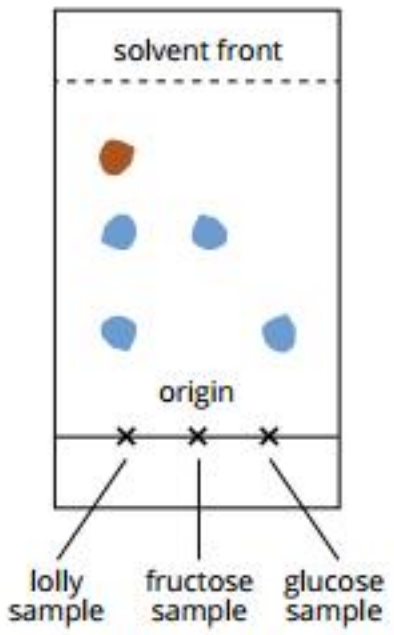


FIGURE 11.5.5 Identification of sugars in a lolly using paper or thin-layer chromatography. The lolly is likely to contain fructose and glucose, as well as a brown-coloured component.

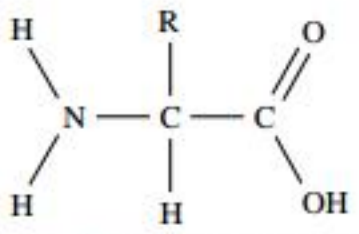


FIGURE 11.5.6 The 20 common amino acids have the same basic structure. The R group is a branched, straight chain, aromatic or other hydrocarbon chain with possible functional group(s). This variation in structure confers the polar or non-polar properties to the molecule.

Method 2: Using standards

In this method, you need to have an understanding of the chemicals that might be present in the sample. The sample is tested on the same chromatogram as pure samples of the possible components in the unknown. These pure samples are known as standards. An example of this strategy is testing a lolly for the presence of glucose and fructose. If spots from the lolly sample move the same distance from the origin as the spots from the fructose and glucose standards, then the lolly is likely to contain the sugars (Figure 11.5.5).

Standards can also be used in paper and thin-layer chromatography as an indication of the amount of a substance present. By applying the standard in a range of concentrations, a visual comparison is made with the sample of interest.

Example: Separation of amino acids by chromatography

Amino acids are the monomers that combine to make all proteins. There are 20 common types, each one containing an acid group (–COOH) and an amine group ($–NH_2$). The generic structure of an amino acid is shown in Figure 11.5.6 and 20 examples are described in your Formula and Data book. The side chains of amino acids, represented by the R group, can be either polar or non-polar. Amino acids can be separated using thin-layer chromatography due to the different polarity of the R groups. Although not coloured, their position on the chromatography plate is revealed using a ninhydrin stain (Figure 11.5.7), applied onto the chromatography slide. This reacts with amino acids to give blue and brown coloured compounds, making them visible in the chromatogram. Figure 11.5.7 shows the chromatography of five pure amino acid samples.

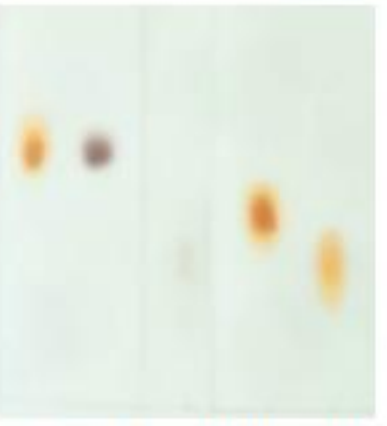


FIGURE 11.5.7 Amino acids separated using silica thin-layer chromatography. The amino acids are colourless and their positions have been revealed using ninhydrin stain.

EXTENSION: COLUMN CHROMATOGRAPHY

Column chromatography uses the same principles as paper and thin-layer chromatography to separate a mixture, but the stationary phase is a three-dimensional porous column structure rather than two-dimensional paper or plate. Column chromatography can be regarded as a simple form of two sophisticated chromatographic techniques: gas chromatography and high-performance liquid chromatography. These techniques give highly accurate results and require very small samples. An example of column chromatography is shown in Figure 11.5.8.

In column chromatography (Figure 11.5.8), the stationary phase consists of small particles loosely packed into a glass or metal column. The sample mixture is applied carefully to one end of the column, and a solvent, which acts as the mobile phase, is dripped onto or pumped through the column from a reservoir above. A tap at the bottom of the column allows the solvent, which is called the **eluent**, to leave the column at the same rate as it enters. Separated components leave the bottom of the column at different times. A record of these times and intensity of detection of each substance is produced as a graph.

As the components are carried down the column, they move between the particles of the stationary phase and are repeatedly adsorbed to the stationary phase and desorbed back into the mobile phase (Figure 11.5.9). The components of the sample undergo the processes of adsorption and desorption to different degrees based on their polarities, so they move at different rates downwards with the eluent. The time each component moves down the column, called the retention time, can be used to identify the individual components.

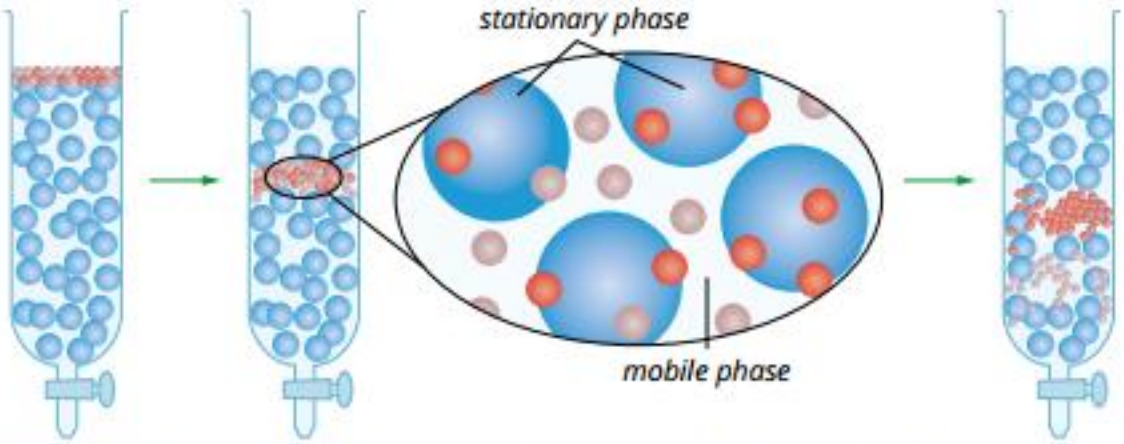


FIGURE 11.5.9 At a molecular level in column chromatography, bonding occurs between the stationary phase and a component in the mobile phase.

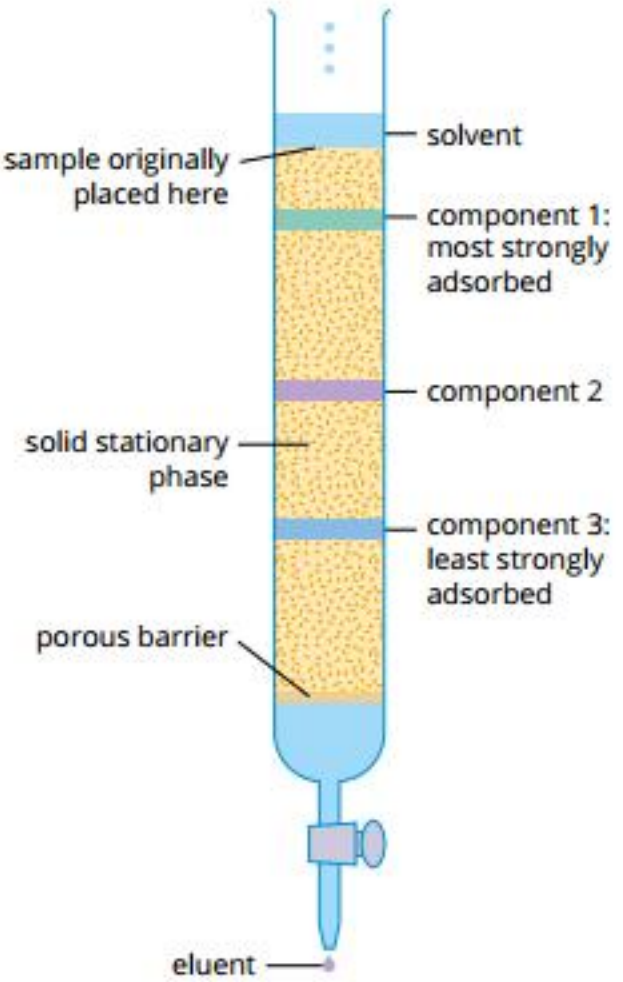


FIGURE 11.5.8 The labelled column shows how components are separated in a mixture using the same principles as paper chromatography.

COMPARING CHROMATOGRAPHIC TECHNIQUES

This chapter has described different chromatographic techniques that can be used for analysis: paper chromatography, thin-layer chromatography and simple column chromatography.

The particular technique chosen depends on a number of factors, including the:

- properties of the components being separated, especially polarity
- amount of sample available for analysis
- concentration of the component in the sample
- sensitivity of the data required
- whether qualitative or quantitative data is required
- time taken for analysis
- cost of equipment.

Chromatography is widely used for the drug testing of blood and urine samples, monitoring water and air pollution, and testing food quality.

11.5 Review

SUMMARY

- Chromatography is a technique commonly used to separate and identify the components in a mixture.
- Paper and thin-layer chromatography are simple forms of this technique.
- All chromatographic techniques involve a mobile phase and a stationary phase.
- Components separate during chromatography because of how strongly they adsorb to the stationary phase and desorb back into the mobile phase.
- Components in a mixture have differing affinities for the mobile and stationary phases due to the differences in polarity of the compounds involved.
- In paper and thin-layer chromatography, the components in a mixture are identified by comparison with known standards and determination of R_f values, where:

$$R_f = \frac{\text{distance the component travels from the origin}}{\text{distance the solvent front travels from the origin}}$$

- Column chromatography also uses these principles and processes in a cylindrical three-dimensional structure.
- In column chromatography, the mobile phase flows through a stationary phase, separating the components and causing them to move down the column.
- When two compounds have very similar interactions with the mobile and stationary phase, they may be able to be separated based on different molecular sizes.
- A component with a similar polarity to the mobile phase (compared to the stationary phase) will have a high R_f value.

KEY QUESTIONS

Describe

1 Identify the correct description for each term.

Term	Description
adsorption	the disruption of the attraction between a substance and the surface to which the substance is adsorbed
desorption	the different compounds in the mixture, which can be separated by chromatography
components	the components of a mixture undergo adsorption to this phase
polar molecule	the attraction of one substance to the surface of another
mobile phase	a molecule that acts as a dipole; it has one or more polar covalent bonds, with the charge being distributed asymmetrically
stationary phase	the solvent that moves through the stationary phase in chromatography

2 Use the following terms to complete the sentences about paper chromatography. Terms can be used more than once.

stationary	mobile	components
origin	phase	sample
above	below	phases

In paper chromatography, the paper acts as the _____ phase. A small spot of a solution is placed at one end of the paper, called the _____. The _____ solution contains a number of different coloured compounds, the _____. The paper is suspended so that the end with the spot is _____ the surface of the solvent. The solvent or _____ phase moves up the _____ phase. Different coloured spots are observed at various places on the paper, due to the separation of different _____ .

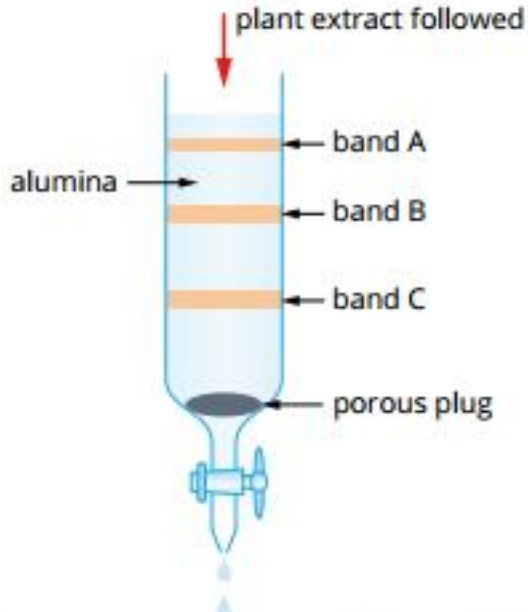
Apply

3 A component moves up a TLC slide at a different rate to the mobile phase. Explain clearly why the R_f value of the component is less than 1.

4 Phenacetin was once an ingredient in analgesic drugs, but it is not used now because it can cause liver damage. It is soluble in chloroform. A chemist wishes to analyse a brand of analgesic by thin-layer chromatography to determine whether it contains phenacetin. Describe the steps in the analysis. (Assume that a sample of pure phenacetin is available to the chemist.)

5 The components in a plant extract were separated by simple column chromatography. The mobile phase used was water and the column was packed with alumina powder. Use the diagram below and the following terms to complete the sentences.

band A	band B	band C
used coarser alumina powder	increased the column length	decreased the column length

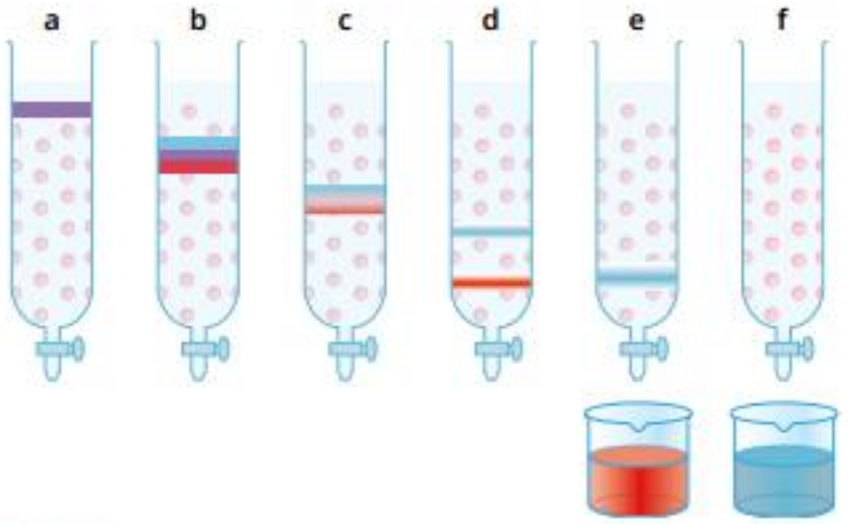


The component most strongly adsorbed to the stationary phase is _____ .
As band B begins to emerge from the column, it appears to separate into two bands. These two components would be more successfully separated if you _____ .

6 For each of the following types of chromatography, determine a possible common material used as the:
- **i** mobile phase
- **ii** stationary phase
  - **a** paper chromatography
  - **b** column chromatography
  - **c** thin-layer chromatography

7 Explain two reasons why the level of the solvent must be below the level of the origin where the samples are placed in paper chromatography.

8 Purple ink is separated using a column containing a polar solvent, as shown in the following figure. Describe the process depicted in the figure.



Analyse

9 Compare the following mixtures: I, II, III, IV:
I–blue ink in a texta; II–the food colour in smarties; III–clay particles in creek water; IV–pigments in water soluble paint.
Which one of the mixtures could not be separated using paper chromatography? Explain why not.

10 Thin-layer chromatography showed that the black dye used in a brand of writing ink contained blue, red, orange and yellow components. The R_f values of these substances in ethanol as solvent are 0.59 (blue), 0.32 (red), 0.80 (orange) and 0.19 (yellow).
- **a** Determine the distance between the blue and yellow components after the solvent front had moved 8.0 cm from the origin.
- **b** Calculate how far the orange component would have travelled when the red component had travelled 6.0 cm from the origin.
- **c** Draw the chromatogram of the ink to scale after the solvent front had moved 15 cm from the origin.

11 Identify any errors in the statements below and, where relevant, suggest a correct statement.
- **a** Mixtures consisting of non-polar components cannot be separated by paper chromatography using a polar stationary phase and a polar mobile phase.
- **b** Components absorb onto the stationary phase.
- **c** When water is used as the mobile phase in paper chromatography, highly polar components will have very small R_f values.

Chapter review

11

KEY TERMS

adsorption
amino acids
asymmetrical molecule
bond angle
bonding electrons
bonding pairs
chromatogram
chromatography
column chromatography
condensation
covalent network solid
desorption
dipole
dipole–dipole forces
dispersion forces
distillation
electric dipole
electron pair arrangement
electron density
electron distribution
electronegativity
electrostatic force
eluent
equilibrium
evaporation
fluoresce
fractional distillation
hydrogen bonding
instantaneous dipole
Lewis structure
lone pair
mobile phase
net dipole
non-polar
non-polar solvent
octet rule
origin
paper chromatography
polar
polar solvent
polarisable
polarised
polarity
polyatomic molecule
pyramidal
qualitative analysis
quantitative analysis
retardation factor (R_f)
solubility
solute
solvent
solvent front
standard
stationary phase
surface tension
symmetrical molecule
temporary dipole
tetrahedral
thin-layer chromatography
trigonal planar
valence electron
valence shell electron pair repulsion (VSEPR) theory
vapour pressure
viscosity
wedge-dash notation

KEY QUESTIONS

Describe

1 Identify the correct bond angle between atoms in a molecule that adopts a tetrahedral shape.
- **A** 180°
- **B** 109°
- **C** 104.5°
- **D** 120°
- **E** 90°

2 Select the correct definition for the electronegativity of an atom.
- **A** the amount of energy required for an atom to lose an electron
- **B** the ability of an atom to form a hydrogen bond
- **C** the ability of an atom to form an ion
- **D** the ability of an atom in a bond to attract bonding electrons to itself

3 Indicate the correct word from the options below to complete the following sentence: Water molecules are predominantly held together in the liquid state by:
- **A** covalent bonds
- **B** hydrogen bonds
- **C** dispersion forces
- **D** ionic bonds

4 Identify the type of intermolecular force that is generally the strongest.
- **A** covalent bonds
- **B** hydrogen bonds
- **C** dispersion forces
- **D** dipole–dipole forces

5 Identify whether each of the following statements about covalent molecular substances is true or false.
- **a** The vapour pressure of a substance is the pressure exerted by a gas in equilibrium with its liquid in a closed container.
- **b** When a substance changes state from a solid to a liquid, the covalent bonds within the molecules are broken.
- **c** A solute will only dissolve in a solvent if their intermolecular forces are very different.
- **d** When a substance changes state from a liquid to a gas, its intermolecular forces of attraction are completely disrupted.

6 State the three main types of intermolecular forces.

7 For hydrogen bonding to occur between molecules, state what group of atoms each molecule must contain.

8 The molecular shape can be different from the electron pair arrangement because:

A electron pairs will always form a trigonal planar shape.

B electron pairs are always non-bonding.

C only the atoms are used to identify the molecule shape.

D the number of electron pairs is always different to the number of covalent bonds.

9 Determine which of the following correctly identifies the shape of these molecules

	CH_2O	NH_3	H_2S
A	trigonal planar	trigonal planar	bent
B	trigonal planar	pyramidal	bent
C	pyramidal	pyramidal	linear
D	pyramidal	pyramidal	linear
E	pyramidal	trigonal planar	linear

10 Identify which of the following is the basis for separation in chromatography.

A interaction of chemicals with both mobile and stationary phases

B movement of chemicals through a column using a carrier gas

C passage of chemicals through a heated column under pressure

D small molecules becoming trapped in gaps between solid particles in a packed column

11 **a** Use the terms 'adsorbed' or 'absorbed' correctly in the sentences below.

i Water was _____ by the towel as the wet swimmer dried himself.

ii A thin layer of grease _____ onto the cup when it was washed in the dirty water.

b State the meaning of the terms 'adsorbed' and 'absorbed'.

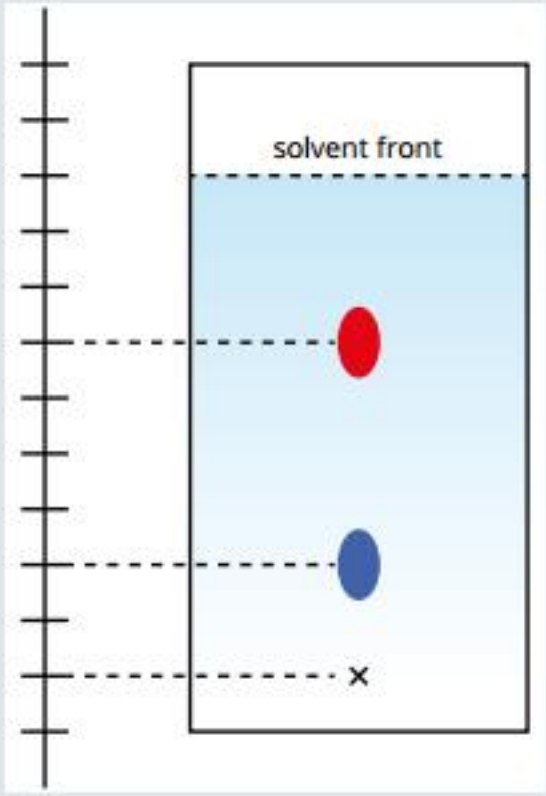
12 Define each of the following terms.

chromatography eluent mobile phase stationary phase

13 Describe how an R_f value is calculated.

14 A sample of brown dye from a lolly is placed at the origin on a chromatography plate. The solvent front moves 9.0 cm from the origin. A blue component of the dye moves 7.5 cm and a red component moves 5.2 cm in the same time. Indicate the R_f values of the two components.

15 The following chromatogram was obtained when mixture X was spotted onto a thin-layer plate and a mobile phase was allowed to run up the slide and was stopped at the dotted line labelled solvent front.



Compared to component A, component B is adsorbed:

A less strongly onto the stationary phase and has a larger R_f value.

B more strongly onto the stationary phase and has a larger R_f value.

C more strongly onto the stationary phase and has a smaller R_f value.

D less strongly onto the stationary phase and has a smaller R_f value.

Apply

16 The melting point of alkanes (hydrocarbon molecules) increases as the number of carbon atoms in the molecule increases because the:

A number of protons increases and therefore the strength of the intermolecular forces decreases.

B number of protons increases and therefore the strength of the intermolecular forces increases.

C number of electrons increases and therefore the strength of the intermolecular forces decreases.

D number of electrons increases and therefore the strength of the intermolecular forces increases.

17 Use your knowledge of VSEPR theory to determine the shape of a molecule that contains a central atom surrounded by four bonding groups of electrons and no lone pairs.

A linear

B trigonal planar

C tetrahedral

D pyramidal

E bent

18 Use your knowledge of VSEPR theory to determine the shape of a molecule that contains a central atom surrounded by three bonding groups of electrons and one lone pair.

A linear
B trigonal planar
C tetrahedral
D pyramidal
E bent

19 Contrast the numbers of bonding pairs and lone pairs of electrons around the central atoms of NCl_3 and CO_2.

20 According to VSEPR theory, the decrease in bond angle as you go from CH_4 to NH_3 to H_2O is due to:

A increasing strength of bonds.
B increasing number of lone pairs.
C decreasing repulsion between hydrogen atoms.
D decreasing size of the central atom.

21 Use the electronegativity values in Figure 11.2.1 on page 273 to calculate the electronegativity difference between the atoms in each of the following covalent bonds and determine which bond is the most polar.

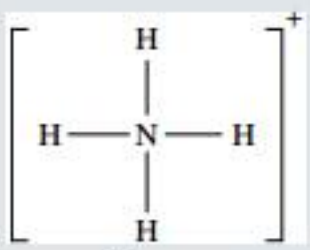
N–N, C–H, H–F, O–F, F–F

22 Calculate the electronegativity differences between the atoms and determine which of the following molecules contains the most polar bond.

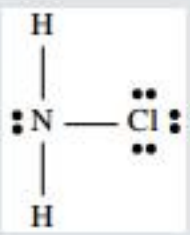
CO_2, H_2O, H_2, H_2S, NH_3

23 All of the following molecules have four pairs of electrons around the central atom. For each one, use your understanding of VSEPR theory to determine whether the molecular shape is tetrahedral, pyramidal or bent.

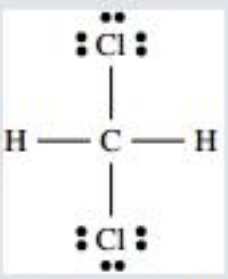
a



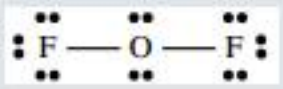
b



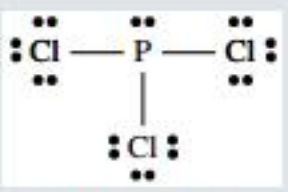
c



d



e



24 Use your understanding of electronegativity and polarity of molecules to determine which of the molecules in Question **23** are polar.

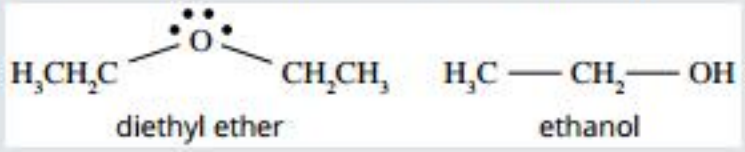
25 In the liquid state, explain what intermolecular forces of attraction exist between molecules of hydrogen chloride (HCl). Draw a representation of these intermolecular forces.

26 Use your understanding of intermolecular forces to identify the type of intermolecular force which must be overcome in each of the following processes.

a the melting of ice
b the conversion of solid iodine to gaseous iodine
c dissolving ethanoic acid (CH_3COOH) in water to make vinegar

27 The following substances increase in boiling point in the order shown: $CH_3F < CH_3Cl < CH_3Br < CH_3I$. Explain this order.

28 Diethyl ether and ethanol are both liquids at room temperature. Explain why ethanol has a lower vapour pressure than diethyl ether at this temperature.



diethyl ether ethanol

29 Select the correct answers from the pairs of words to complete the paragraphs about chromatography.

Chromatography is a technique used to *separate/ destructively analyse* the various compounds in a mixture. Simple chromatography methods, such as paper and thin-layer chromatography, are *quick and inexpensive/accurate and efficient* and provide *qualitative/quantitative* results for determining the *identity/concentration* of components present in the mixture, whereas more sophisticated chromatographic techniques enable the *qualitative/quantitative* determination of the components of a mixture.

All techniques involve the movement of a mobile phase over a stationary phase. Separation occurs due to the *adsorption/desorption* of components onto the stationary phase and *adsorption/desorption* and dissolving of components into the mobile phase. The rate at which the components move along with the mobile phase over the stationary phase depends mainly on their *size/polarity* with respect to *the stationary phase/ the mobile phase/both stationary and mobile phases.*

30 Use the following terms to complete the summary of column chromatography. Not all terms are used.

mobile	adsorb	desorb
longest	shortest	stationary

During column chromatography, the components of the sample _____ onto the stationary phase and _____ into the liquid mobile phase. A component that adsorbs most strongly to the _____ phase and is least soluble in the _____ phase would be expected to take the _____ time to pass through the column.

The following information refers to Questions 31 and 32.

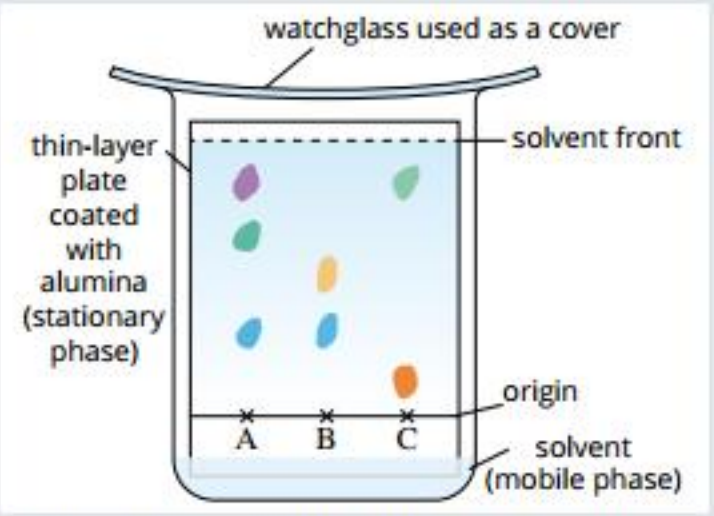
Paper chromatography was used to separate the pigments in a plant leaf. The pigments were extracted from the leaf using ethanol and a spot of the pigment mixture was placed on a sheet of chromatography paper. Spots of pure pigments that are likely to be present in the leaf were also placed on the paper beside the spot of the mixture. The chromatogram was performed inside a closed jar that was partly filled with ethanol.

31 Select which one of the following options is the mobile phase in this instance.

A pigments
B ethanol
C paper
D ethanol vapour in the closed jar

32 Explain how you could compare the components and the standards and determine which standards were present in the mixture.

33 Consider the paper chromatography shown below.



a Determine how many different components are present in sample B.
b Determine which component of colour A is least strongly adsorbed on the stationary phase.
c Identify which samples are likely to have one component in common.
d The green spot in sample A is 8.0 cm above the origin. The R_f value of this green spot is 0.74. The orange and green spots of sample C are 3.0 cm and 9.0 cm above the origin respectively. Calculate the R_f values of each component of sample C. Give your answer to 2 significant figures.

34 Consider the paper chromatogram in Question **33**.

a Describe why the level of the solvent must be lower than the origin where spots of the mixture are originally placed.
b Explain why R_f values are always less than one.
c Determine how many different components are shown on the chromatogram.

Analyse

35 Polarity (a dipole) in a covalent bond is a result of:

A the tetrahedral shape of the molecule.
B bonding between a metal atom and a non-metal atom.
C bonding between atoms of different size.
D electronegativity difference.

36 List the following substances in order of increasing polarity

CH_4 CH_3Cl CH_3F CF_4

37 Determine which of the following would be expected to show hydrogen bonding:

H_2O CH_4 SiH_2Cl_2 NH_3 CF_4

38 Draw the Lewis diagrams of the following molecules and apply your understanding of VSEPR theory to determine their molecular shape.

a PF_3
b NH_3

39 Determine the bond angles in each of the following molecules using your understanding of VSEPR theory.

a CF_4
b CO_2
c H_2O
d NH_3

40 Predict the shape of each of the following molecules.

a CS_2
b H_2S
c SiH_4

41 Identify which of the following statements about intermolecular forces is FALSE (choose all that apply).

A Intermolecular forces involve two atoms sharing a pair of electrons.
B Intermolecular forces can be hydrogen bonding, dipole–dipole bonding or dispersion forces.
C Intermolecular forces are due to electrostatic attraction of two oppositely charged regions.
D Intermolecular forces dictate the physical properties of a substance.
E The higher the intermolecular forces, the lower the melting point and boiling points.

42 Determine which of the following statements about the structure of CO_2 is correct.

A All the atoms are joined by relatively strong network bonds.
B It consists of molecules with intermolecular bonding within them and intramolecular forces between them.
C It consists of a lattice of ions.
D It consists of an array of molecules held together by dispersion forces.
E It consists of an array of molecules held together by dipole–dipole bonding.

43 Consider the polarity of the bonds and the shapes of the following molecules and predict which molecules are polar.
- **a** CH_2Cl_2
- **b** NF_3
- **c** Cl_2
- **d** HCl
- **e** N_2

44 Predict which molecule would be the most polar: NH_3 or PH_3. Explain your choice.

45 Consider the two compounds CH_4 and CCl_4. CH_4 is a gas at room temperature, whereas CCl_4 is a liquid.
- **a** Determine which substance has the stronger intermolecular forces of attraction.
- **b** Compare the structure of the molecules in each substance and use this comparison to explain the difference in the strengths of the intermolecular forces.

46 Classify the following compounds in order of increasing strength of the intermolecular forces of attraction present in each: F_2, HF, HCl. Explain your order.

47 Consider the two compounds OF_2 and CF_4. OF_2 has a boiling point of −145°C and CF_4 has a boiling point of −128°C. From their boiling points, determine which compound contains the strongest intermolecular forces of attraction. Compare the structure of the molecules in each compound and discuss why their boiling points differ.

48 Hydrogen bonding occurs in both NH_3 and H_2O. Predict the substance in which the hydrogen bonding would be stronger. Explain your answer and use a diagram to illustrate your point.

49 Fluorine (F_2) is a gas at room temperature, whereas iodine (I_2) is a solid. Identify which factor best explains this difference using your understanding of intermolecular forces.

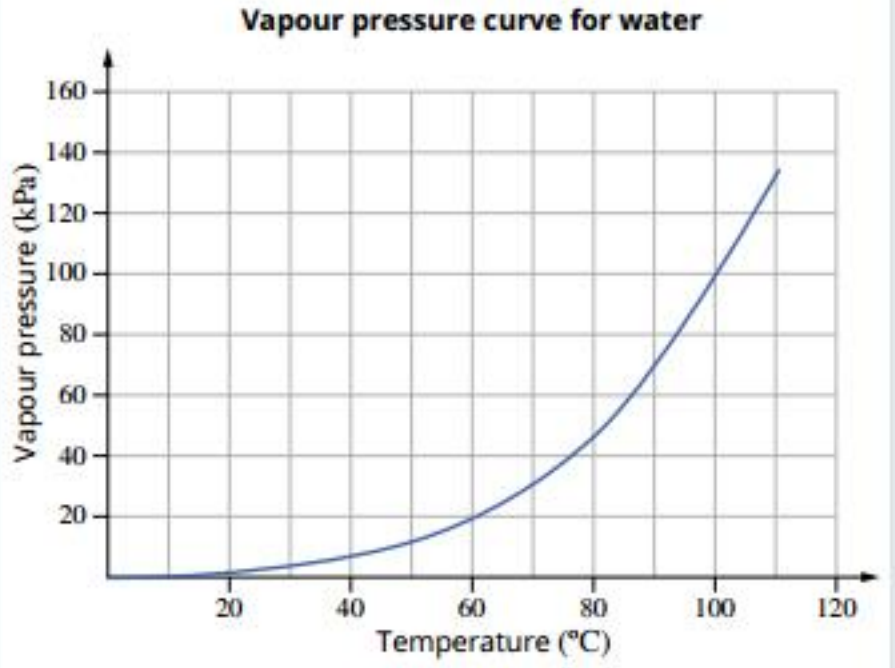
50 Predict which of the following substances would have the highest boiling point: CO_2 or NO_2. Explain your choice.

51 Ammonia (NH_3) boils at −33°C, whereas hydrazine ($H_2N–NH_2$) boils at 114°C. Explore a possible reason for the very large difference in boiling points.

52 Predict which substance would have the lower vapour pressure at a given temperature: CH_2F_2 or CH_4. Explain your choice.

53 Predict which gas would have the highest solubility in water: N_2, Cl_2, CO_2, NH_3.

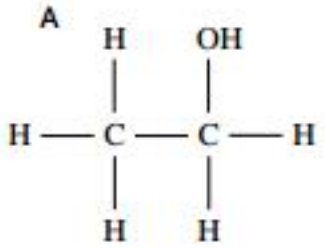
54 The vapour pressure curve for water is shown in the graph below. Use this graph to answer the questions that follow.



- **a** Determine why the vapour pressure of water increases with temperature.
- **b** State the normal boiling point of water.
- **c** Predict the boiling point of water on the summit of Mount Everest where the atmospheric pressure is only about 35 kPa.
- **d** Explore why the boiling point of water is so much lower on the summit of Mount Everest than at sea level.

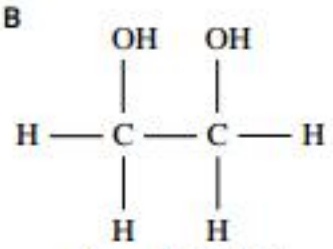
55 A student recorded the boiling points of four different covalent molecular substances but forgot to write down the substance that corresponded with each boiling point. The student tested ethanol, ethane-1,2-diol, methanol and propan-1-ol (Lewis diagrams shown on the next page). Analyse the molecular structure of each substance and use your understanding of intermolecular forces to match each substance with its correct boiling point.

A



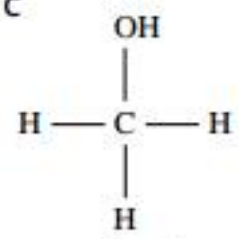
ethanol

B



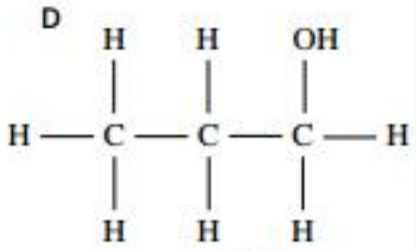
ethane-1, 2-diol

C



methanol

D



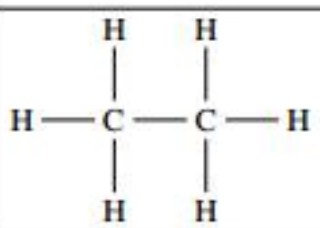
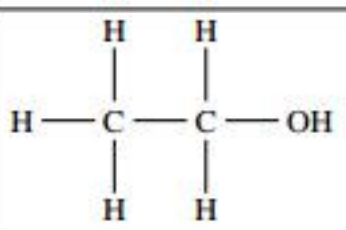
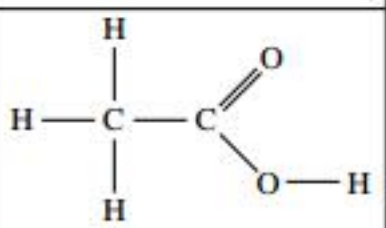
propan-1-ol

Substance	Boiling point (°C)
?	64.5
?	78.5
?	97.2
?	198

56 Analyse the data in the table below and explore the evidence that allows you to conclude that methylamine, CH_3NH_2, has stronger intermolecular forces of attraction than chloromethane, CH_3Cl.

Substance	Molecular formula	Melting point	Boiling point	Solubility in water
methylamine	CH_3NH_2	–92.5	–6.3	very soluble
chloromethane	CH_3Cl	–97.7	–23.8	sparingly soluble

57 The table below shows the structural formulas of three compounds (ethane, ethanol and ethanoic acid) and their solubility in the non-polar solvent hexane. Their melting points are below 0°C.

Compound	Structural formula	Solubility in hexane
ethane		soluble
ethanol		mostly insoluble
ethanoic acid		insoluble

a Choose a compound from the table that you would expect to be soluble in water. Provide a reason.

b Categorise the molecules in the above table as polar or non-polar.

58 A dielectric constant is a measure of the polarity of a compound. A high dielectric constant refers to a polar compound. Using the data presented below, identify the position of the following compounds on a paper chromatogram using water as the solvent. Present your answer in the order of highest R_f value to lowest R_f value.

Name	Structure	Dielectric constant
hexane	$CH_3(CH_2)_4CH_3$	2.02
1-butanol	$CH_3CH_2CH_2CH_2$–OH	17.8
1-propanol	$CH_3CH_2CH_2$–OH	20.1
ethanol	CH_3CH_2–OH	24.3
methanol	CH_3–OH	33.0
acetonitrile	H_3C–C≡N	36.6

59 Compare the rates of adsorption and desorption for a component that appears at the top of a paper chromatogram to the rates for a component that appears at the bottom of the chromatogram.

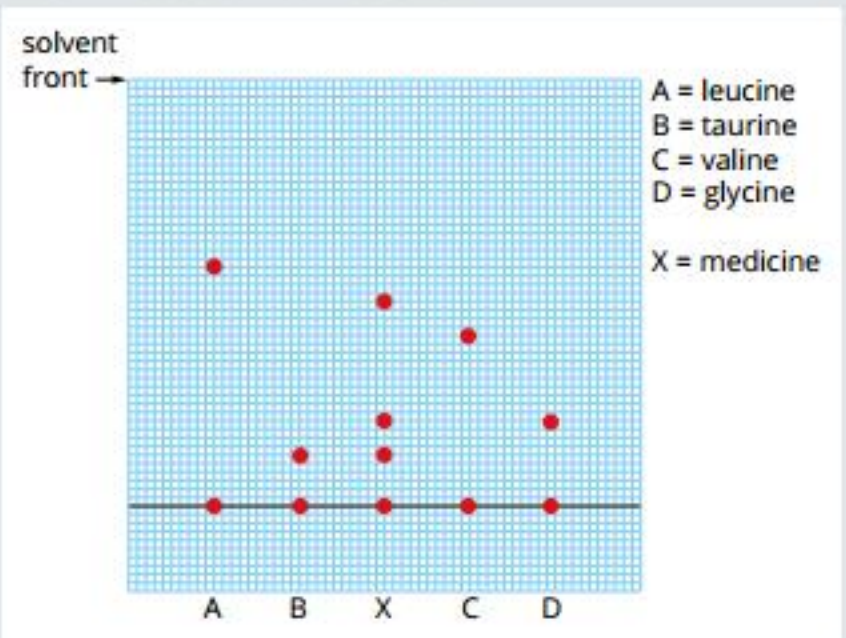
60 An extract from a plant was analysed by thin-layer chromatography with a non-polar solvent. The chromatogram obtained is shown in the following diagram. The following table gives the R_f values of some chemicals commonly found in plants measured under the same conditions.

Chemicals found in plants	R_f
xanthophyll	0.67
β-carotene	0.82
chlorophyll a	0.48
chlorophyll b	0.35
leutin	0.39
neoxanthin	0.27

Measure and record the distance from the origin to the centre of each band, and to the solvent front. Use these values to:

- **a** calculate the R_f value of each band.
- **b** compare R_f values for the bands with the R_f values provided and name the chemicals present in the extract.
- **c** explain if the chromatogram would have appeared similar if water had been used as the solvent.

61 The diagram below shows a thin-layer chromatogram of amino acids in a medicine.



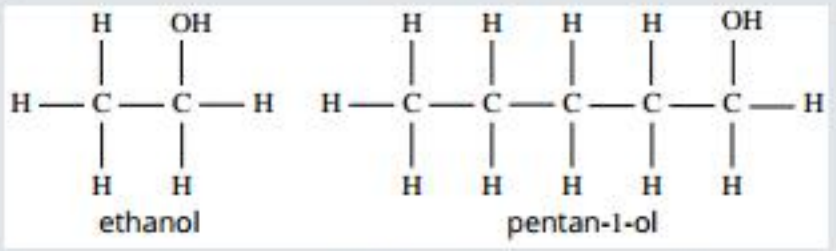
- **a** Identify which amino acids are in the medicine.
- **b** Amino acids are colourless. Determine what technique could be used to make the amino acid spots visible.
- **c** Analyse which amino acid is bonded least strongly to the stationary phase.

62 Explain the key stages in the thin-layer chromatography procedure used to produce the chromatogram shown in the previous question.

Interpret

63 VSEPR theory recognises the significant effect that lone pairs of electrons have on the shapes of molecules such as water. If the lone pairs of electrons *were not* taken into account, predict what might be expected for the shape of a water molecule. Consider this predicted shape for a water molecule again: discuss how the observed properties of water would confirm that this shape is incorrect.

64 Consider the structures of ethanol and pentan-1-ol as shown below. Both substances are polar and contain hydrogen bonds in the liquid state. Ethanol is highly soluble in water (which you would expect for a substance that contains hydrogen bonds), whereas pentan-1-ol is only very slightly soluble. Explore a possible reason for this difference.

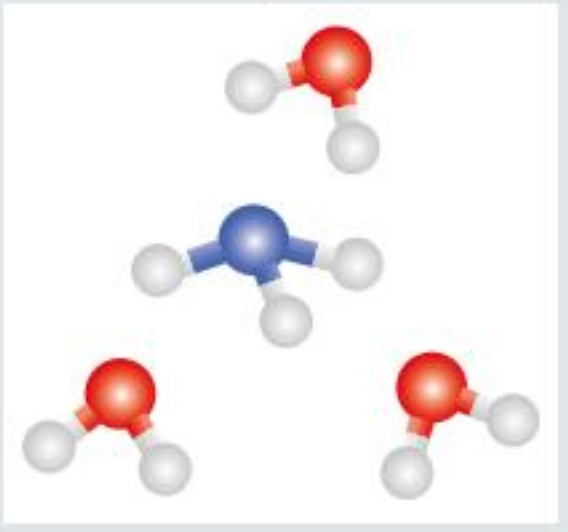


65 When water freezes at 0°C, the ice it forms can float on the liquid water. However, when benzene (C_6H_6) freezes at 5.5°C, the frozen benzene cannot float on the liquid benzene; instead, it sinks to the bottom. Propose a possible reason for this difference.

66 Using a molecular model kit or plasticine and plastic straws, make the molecules mentioned in Table 11.1.1 on page 268. Identify the positioning of the lone pairs and the effect of these of the bond angles in the molecule.

67 The diagram below shows the dissolving of NH_3 in water but all labels for atoms and partial charges have been removed.

- **a** Label the diagram to show all atoms and partial charges on molecular dipoles.

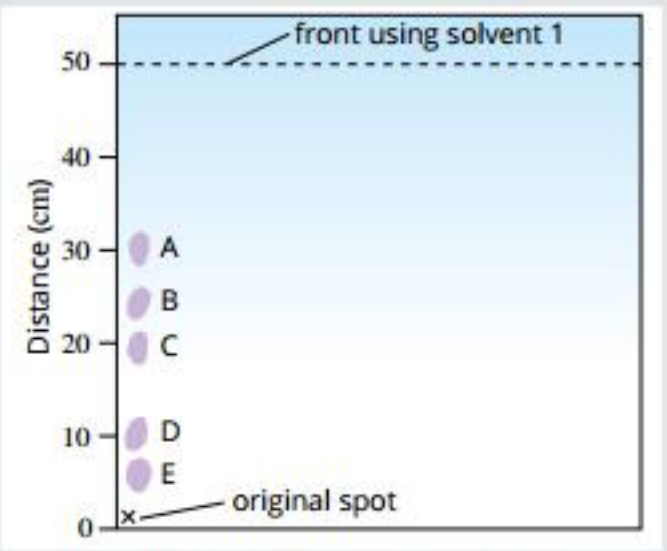


- **b** Describe the solubility of NH_3. Justify your response by referring to the interactions shown in the diagram.

68 The amino acids present in a sample of fruit juice can be detected by thin-layer chromatography. R_f values of some amino acids in two separate solvents are given in the table below.

Amino acid	Solvent 1 R_f	Solvent 2 R_f
lysine	0.12	0.55
leucine	0.58	0.82
proline	0.39	0.88
valine	0.40	0.74
2-aminobutyric acid	0.28	0.58
threonine	0.21	0.49
hydroxyproline	0.21	0.67
β-phenylamine	0.50	0.86
isoleucine	0.57	0.81
alanine	0.24	0.55
serine	0.19	0.34
glutamic acid	0.25	0.33
glycine	0.20	0.40
arginine	0.13	0.60
taurine	0.12	0.33
tyrosine	0.38	0.62

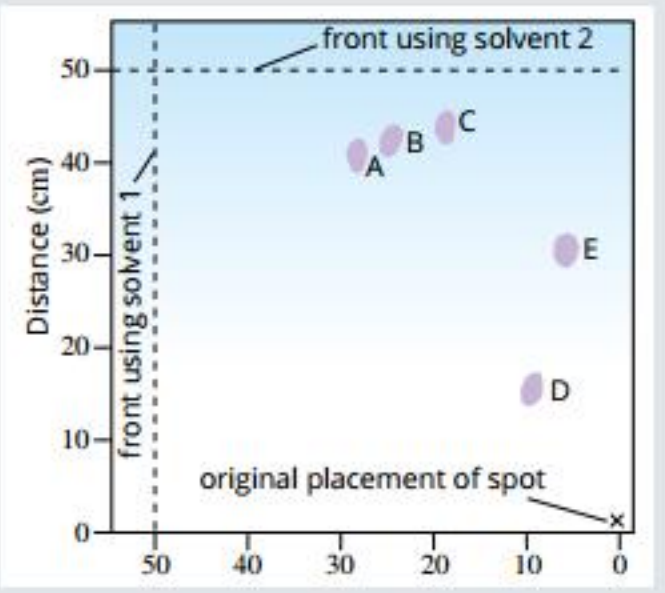
To achieve better separation of the complex mixture of substances present in the juice, a 'two-way' chromatogram was prepared. The first step in this procedure was to run a chromatogram using solvent 1. The results of this chromatogram are shown in the following figure.



a Calculate the R_f value of each spot on the chromatogram.

b Determine the amino acids responsible for each spot. Indicate if you consider that there could be more than one possibility.

The TLC plate was then turned around anticlockwise so that it lay at a right angles to the original and a second chromatogram was produced using solvent 2. This figure shows the appearance of the TLC plate after some time.



c Use the table to identify each component in the mixture.

d Propose a possible advantage of a two-way chromatogram.

69 The following materials are commonly used in chromatography: water, butanol, paraffin wax, glass sheets, paper strips, powdered alumina plates and hexane. Research amino acid identification and choose a suitable stationary phase and mobile phase from the list to use in the analysis of amino acids by thin-layer chromatography.

70 Some polar substances in blood and urine can be detected using a 'dipstick' test. The test stick is dipped into the sample and the assay is completed as the water-based fluid is drawn up the stick. Determine how a thin-layer chromatography version could be used to separate the polar compound of interest from unrelated substances in the mixture and then tested for its presence.

Data analysis

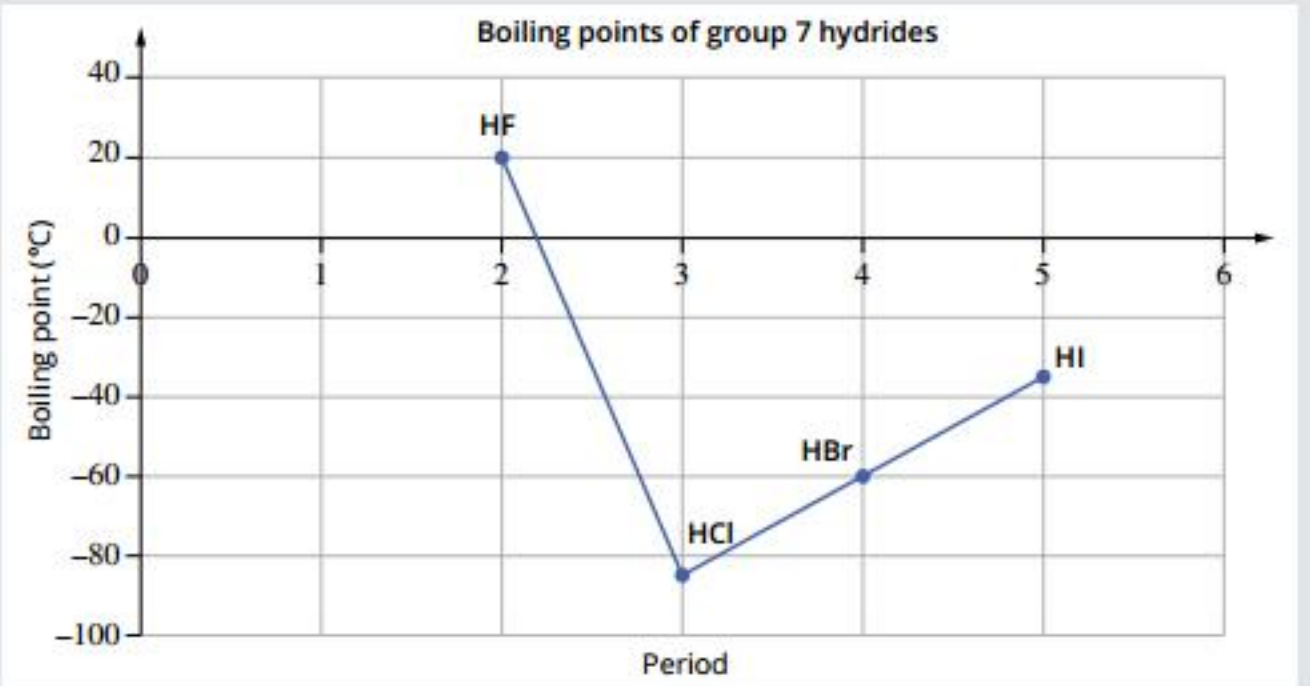
DATA SET 1

The information below applies to Questions 1–4.

The boiling points of group 17 hydrides are shown in the table and graph below.

Table 1 Boiling points of group 17 hydrides

Compound	Boiling Point (°C)
HF	20
HCl	−85
HBr	−60
HI	−35
HAt	



Question 1 (2 marks)

Identify a trend, including an exception to this trend.

Question 2 (1 mark)

Using the data from Table 1, **calculate** a possible value for the boiling point of HAt. Give your answer to the nearest whole number.

Question 3 (1 mark)

Sequence the compounds in order of intermolecular bonding strength from weakest to strongest bonds.

Question 4 (2 marks)

Infer the main type of intermolecular forces present in **each compound** that has caused the observed trend(s).

CHAPTER

12 Gases

Gases are one of the three fundamental states of matter, and they have fascinated scientists for centuries due to their unusual properties. Unlike the other two states, liquid and solid, the particles in gases have more kinetic energy. This allows the particles to be much further apart which, as you will find reading through this chapter, accounts for many of their important and unique characteristics.

In this chapter, you will explore the properties of gases and relate these to kinetic theory. You will learn how the temperature, pressure and volume of a gas are measured, and how the volume of a gas can be calculated from its amount measured in moles. You will also learn how to perform stoichiometric calculations relating to gases.

Syllabus subject matter

Topic 1 • Intermolecular forces and gases

■ GASES

- State the relationship between the volume of a gas, number of moles and molar volume at standard temperature and pressure (STP). **12.2**
- Apply the kinetic theory of gases to explain the relationships between pressure, temperature, and volume of a gas. **12.1**
- Identify that the kinetic theory of gases applies to ideal gases. **12.2**
- Apply the ideal gas equation to calculate the mass of chemicals and/or the volume of a gas (STP) involved in a chemical reaction.
  (Formula: $PV = nRT$) **12.3**
- Analyse data to determine the relationships between pressure, temperature and volume of a gas. **12.2**

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12.1 Introducing gases

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the properties of gases
- explain the properties of gases using kinetic theory
- explain the relationship between pressure, temperature and volume of a gas, using kinetic theory
- perform calculations to convert units of volume and temperature.

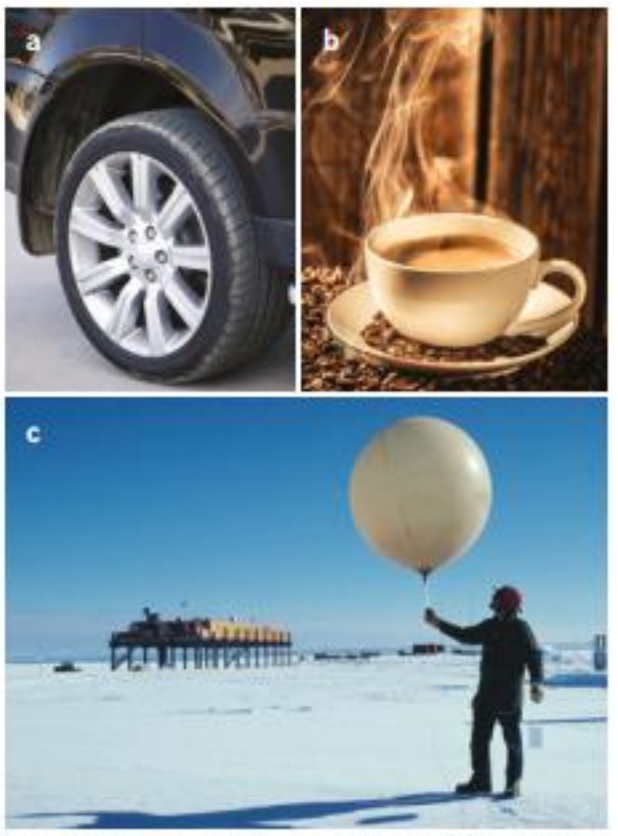


FIGURE 12.1.1 (a) Air is used to inflate vehicle tyres. (b) The movement of gases causes the smell of a freshly brewed cup of coffee to rapidly fill an entire room. (c) This weather balloon is only partially inflated when released to collect data. Its volume increases because of pressure changes as it ascends into the atmosphere.

Under the right conditions of **pressure** and temperature, most substances can exist as a **gas**. Every day you observe the behaviour of gases (Figure 12.1.1). Air is a mixture of gases and is easily compressed. When the car goes over a bump in the road, the air in the tyres compresses slightly and absorbs the impact of the bump (Figure 12.1.1a). Gases mix readily and, unlike solids and liquids, occupy all available space (Figure 12.1.1b). The volume of a gas increases because of pressure changes as it ascends into the atmosphere (Figure 12.1.1c). Such examples can tell you a great deal about the physical properties of gases—those properties that can be observed and measured without changing the nature of the gas itself.

In this module, you will learn about the properties and behaviour of gases.

PROPERTIES OF GASES

The physical properties of gases were introduced in Chapter 10, and each of the examples shown in Figure 12.1.1 can be explained by these properties. Gases assume the volume and shape of their container (Figure 12.1.2), and two gases will mix evenly and completely when placed in the same container. This suggests that the particles move independently of one another. The low **density** of gases, relative to that of liquids and solids, is because the particles in a gas are much more widely spaced apart. This allows gases to be the most compressible form of matter.

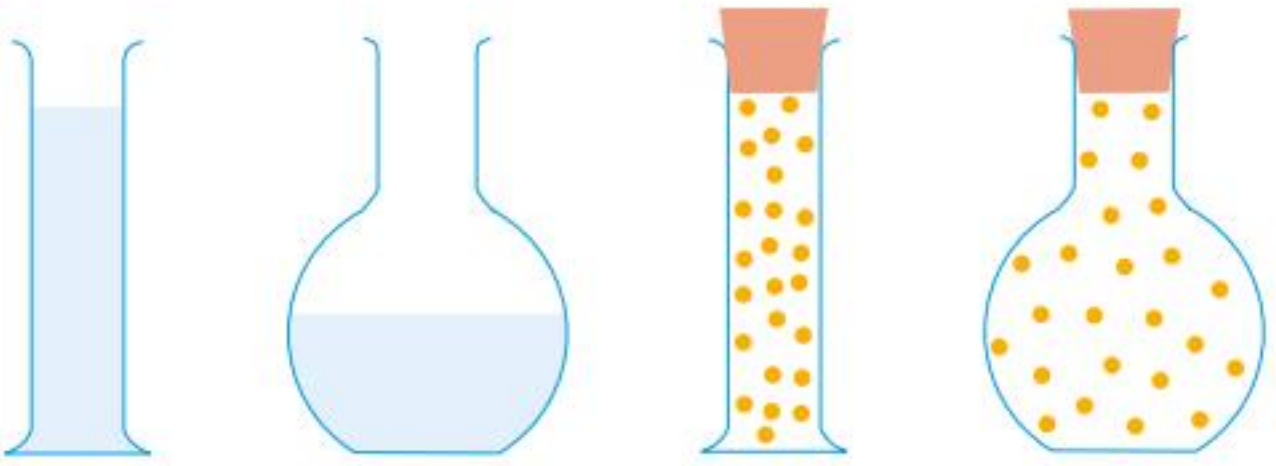


FIGURE 12.1.2 Both liquids and gases take the shape of the container they are in. However, a liquid has a fixed volume, whereas the volume of a gas expands to fill all available space in a container.

Gases assume the volume and shape of their container, are the most compressible form of matter, mix evenly and completely when confined to the same container, and have much lower densities than liquids and solids.

The properties of gases compared to the properties of solids and liquids are summarised in Table 12.1.1. These observations can be used to develop a model of gas behaviour.

TABLE 12.1.1 Some properties of the three states of matter

	Gases	Liquids	Solids
Density	low	high	high
Volume and shape	fill the space available; particles move independently of one another	fixed volume, adopt shape of container; particles are affected by attractive forces	fixed volume and shape; particles are affected by attractive forces
Compressibility	compress easily	almost incompressible	almost incompressible
Ability to mix	mix together rapidly	mix together slowly unless stirred	do not mix unless finely divided

KINETIC THEORY

The properties of gases can be explained using **kinetic theory**. Kinetic theory is described in Chapter 10, and states that all matter consists of particles in motion, and as the temperature increases, the movement of the particles increases.

According to this theory:

- gases are composed of small particles, whether atoms or molecules
- the volume of the particles in a gas is very small compared with the volume they occupy. Consequently, most of the volume occupied by a gas is empty space
- gas particles move rapidly in random, straight-line motion
- particles collide with each other and with the walls of the container
- the forces between particles are extremely weak
- kinetic energy is the energy of motion. The average kinetic energy of gas particles increases as the temperature of the gas increases.

Gases are composed of small particles, either atoms or molecules. These particles are very small compared to the volume of the container, so most of the volume occupied by a gas is actually empty space. This is not the case with liquids and solids. In liquids and solids, the particles are more closely associated with one another and have very little space between them. For this reason, gases have comparatively low density and are much more compressible.

The **intermolecular forces** between gas particles are extremely weak and are easily overcome by the kinetic energy of the molecules. As a result, gas particles tend to move in an independent manner. They have a rapid, random and straight-line motion, colliding with one another and the sides of the container. This explains why gases have the property of assuming the shape and volume of their container.

Kinetic energy (KE) is the energy of motion. The kinetic energy of a particle is calculated from the formula:

$$\text{KE} = \frac{1}{2}mv^2$$

where KE is in joules, mass (m) is in kilograms, and velocity (v) is in metres per second.

In a gas, when particles collide, the kinetic energy of the gas particles can be transferred from one particle to another, but the total kinetic energy remains constant. Therefore, collisions between gas particles are described as **elastic collisions**—collisions where kinetic energy is conserved. According to kinetic theory, as the temperature of the particles increases, so does their speed. This means the particles at a higher temperature have more kinetic energy when they move around and collide with each other and the sides of their container. This influences both the volume and pressure of a gas.

FIGURE 12.1.3 A balloon filled with air at room temperature is dipped into liquid nitrogen at −196°C. The volume of the air inside the balloon decreases dramatically.

FIGURE 12.1.4 Pumping more air into a tyre increases the pressure in the tyre because more particles are being pumped into a nearly fixed volume.

TEMPERATURE, VOLUME AND PRESSURE OF GASES

There is a relationship between the volume, pressure, temperature and amount of a gas. For example, when you blow up a balloon, the balloon expands because you put more air into it and the rubber of the balloon stretches. As you add more gas particles, the gas increases in volume. If you then plunge that balloon into liquid nitrogen, as shown in Figure 12.1.3, the balloon shrinks dramatically. The kinetic energy of the particles decreases as the temperature decreases. This means that the particles move more slowly and are condensed into a smaller volume. Pumping more air into a tyre, as shown in Figure 12.1.4, increases the pressure inside the tyre. The volume of the tyre is fixed, so adding more gas particles means there will be more collisions with the walls of the tyre, and this means an increase in pressure. You will further investigate the mathematical relationship between the pressure, temperature, volume and amount of a gas in the next module (12.2).

Volume

Volume is the quantity used to describe the space that a substance occupies. Because a gas occupies the whole container that it is in, the volume of a gas is equal to the volume of its container.

There are several different units used for volume, some of which are represented in Figure 12.1.5. The common units are litre (L), millilitre (mL), cubic decimetre (dm^3) and cubic centimetre (cm^3). Small volumes of gas are usually measured in millilitres (mL) or litres (L). Very large samples are measured in cubic metres (m^3).

- $1\ dm^3 = 1 \times 10^{-3}\ m^3 = 1 \times 10^3\ cm^3 = 1\ L$

It is helpful to remember that

- $1\ dm^3 = 1\ L$, and
- $1\ cm^3 = 1\ mL$

Note: 1 decimetre (dm) is 10 centimetres (cm).

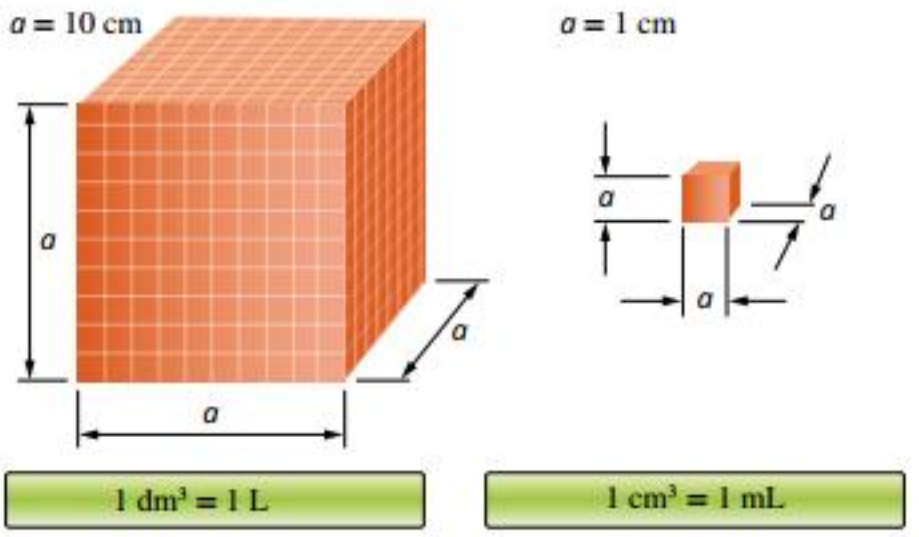


FIGURE 12.1.5 Cubic centimetres, millilitres and litres are the most commonly used units of volume.

Worked example 12.1.1

CONVERTING VOLUME UNITS

A gas has a volume of 255 mL. Calculate its volume in:

a cubic centimetres (cm^3)

b litres (L)

c cubic decimetres (dm^3).

Thinking	Working
Apply the conversion factors for each of the units of volume. Apply the correct conversion to each situation.	**a** The units of mL and cm^3 are equivalent. $1\,mL = 1\,cm^3$ $255\,mL = 255\,cm^3$ **b** $1000\,mL = 1\,L$ $\text{new volume} = 255\,mL \times \frac{1\,L}{1000\,mL}$ $= 0.255\,L$ **c** $1 \times 10^3\,cm^3 = 1\,dm^3$ $1\,cm^3 = 1\,mL$ Therefore, $255\,mL = 255\,cm^3$. $\text{new volume} = 255\,cm^3 \times \frac{1\,dm^3}{1 \times 10^3\,cm^3}$ $= 0.255\,dm^3$

➤ Try yourself 12.1.1

CONVERTING VOLUME UNITS

A gas has a volume of 700 mL. Calculate its volume in:

a cubic centimetres (cm^3)

b litres (L)

c cubic decimetres (dm^3).

Pressure

Pressure is the force exerted on any surface compared to the area of the surface. Gases exert pressure on any surface they come into contact with. This is because the constant motion of the particles results in collisions with that surface.

The more a gas is compressed, the more frequently the gas particles collide with each other and the walls of their container. The increased frequency of collisions with the walls of the container increases the force on the walls of the container. The force per unit area is the pressure.

Air is a mixture of gases including nitrogen, oxygen, carbon dioxide and argon. In the air in a container, the nitrogen molecules collide with the walls of the container, exerting a pressure. In a similar way, the oxygen molecules exert a pressure, as do molecules of the other gases present in the mixture. In the gaseous mixture of nitrogen and oxygen shown in Figure 12.1.6 on page 320, the measured pressure is the sum of the partial pressure of oxygen and the partial pressure of nitrogen.

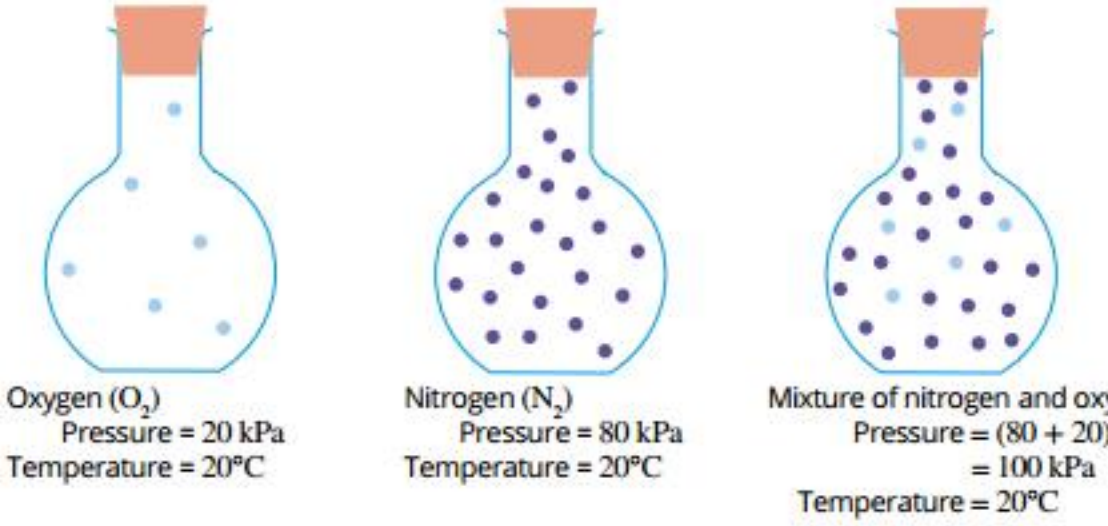


FIGURE 12.1.6 The total pressure of a mixture of gases is the sum of the partial pressures (individual pressures) of each of the gases in the mixture.

The units of pressure depend on the units used to measure force and area. Over the years, scientists in different countries have used different units to measure force and area, so there are a number of different units of pressure.

The Système international (SI) unit for force is the newton (N) and the SI unit for area is the square metre (m^2); therefore, the SI unit of pressure is newtons per square metre ($N\ m^{-2}$). One newton per square metre is equivalent to a pressure of 1 **pascal** (Pa). This is known as an SI derived unit.

Historically, the use of mercury barometers resulted in pressure often being measured in millimetres of mercury, or mmHg. When filling up your car tyres, you may notice another unit of pressure, PSI, which stands for pounds per square inch. 100 kPa is approximately 12.5 PSI.

Another unit for pressure is the **standard atmosphere** (atm). One standard atmosphere (1 atm) is the pressure required to support 760 millimetres of mercury (760 mmHg) in a mercury barometer at 25°C. This is the average atmospheric pressure at sea level. One atmosphere is approximately 100 kPa, and this is the value that is used to represent a standard pressure on Earth.

The units of gas pressure that you are likely to use are summarised in Table 12.1.2.

TABLE 12.1.2 Common units of gas pressure

Name of unit	Symbol for unit	Conversion to Pa (or kPa)
newtons per square metre	$N\,m^{-2}$	
pascal	Pa	$1\,N\,m^{-2} = 1\,Pa$
kilopascal	kPa	$1\,kPa = 1 \times 10^3\,Pa$

These relationships can be used to convert pressure from one unit to another.

Temperature

Kinetic molecular theory describes how increasing the temperature of a gas increases the average kinetic energy of the gas particles. Temperature is therefore an important quantity when describing a gas.

Table 12.1.3 shows the results of an experiment that investigates the relationship between temperature and the volume of a given amount of any gas. In this experiment, the gas in a syringe is heated slowly in an oven. The plunger of the syringe is able to move freely, which keeps the pressure constant.

TABLE 12.1.3 Variation of volume with temperature

Temperature (°C)	20	40	60	80	100	120	140
Volume (mL)	60.0	64.1	68.2	72.3	76.4	80.5	84.6

The graph of these results is linear, as shown in Figure 12.1.7. When the graph is extrapolated to a volume of 0 L, it crosses the temperature axis at −273°C. If the origin is reset at −273°C, this graph passes through the origin. This is what led scientists to develop the **Kelvin scale**, described in Chapter 10. On the Kelvin scale, one temperature increment is equal to one temperature increment on the Celsius scale, and 0°C is equal to 273 K.

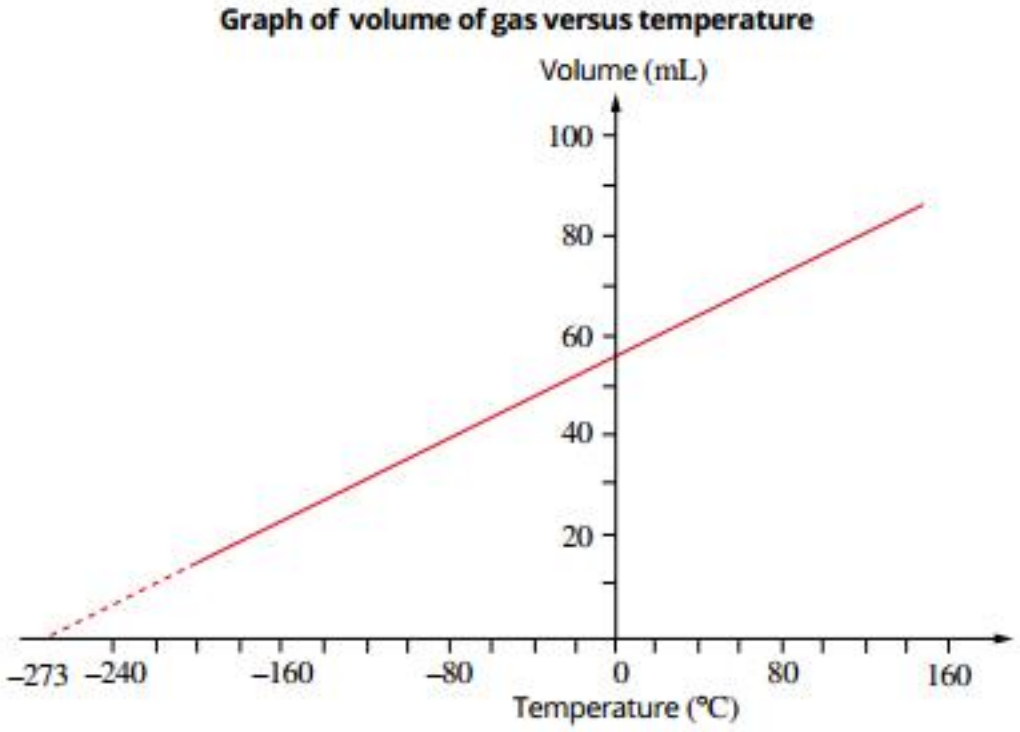


FIGURE 12.1.7 The variation of volume with temperature for a fixed amount of gas at constant pressure

The relationship between temperature on the Celsius scale and temperature on the Kelvin scale is given by the equation:

$$T \text{ (in K)} = T \text{ (in °C)} + 273$$

The temperature 0 K (−273°C) is the lowest temperature theoretically possible. For this reason, 0 K is known as absolute zero (Figure 12.1.8). At this temperature, all molecules and atoms have minimum kinetic energy. The Kelvin scale has no degree sign—the unit is written as just K.

Worked example 12.1.2

CONVERTING TEMPERATURES FROM CELSIUS TO KELVIN

Calculate 300°C on the Kelvin temperature scale.	
Thinking	**Working**
T (in K) = T (in °C) + 273	T (in K) = T (in °C) + 273 = 300 + 273 = 573 K

➤ Try yourself 12.1.2

CONVERTING TEMPERATURES FROM CELSIUS TO KELVIN

Calculate 100°C on the Kelvin temperature scale.

T (in K) = T (in °C) + 273

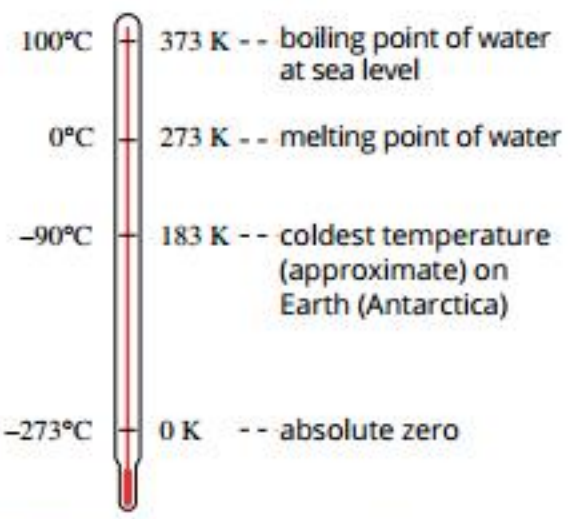

100°C
373 K - - boiling point of water at sea level
0°C
273 K - - melting point of water
–90°C
183 K - - coldest temperature (approximate) on Earth (Antarctica)
–273°C
0 K - - absolute zero

FIGURE 12.1.8 The Celsius and Kelvin temperature scales.

12.1 Review

SUMMARY

- Gases are one of the fundamental states of matter.
- Gases have these physical properties:
  - They have low density.
  - They assume the shape and volume of their container.
  - They compress easily.
  - They mix together rapidly.
- The properties of gases can be understood using kinetic theory.
  - The particles in gases are constantly in motion.
  - The particles move independently, which is why gases assume the shape and volume of their container and mix easily.
  - There is a comparatively large amount of empty space between the particles of gases, which is why they compress easily and are low in density.
- Volume is the quantity used to describe the space that a gas occupies.
- There are several different units used for volume of gases. The common units are litre (L), millilitre (mL), cubic decimetre (dm^3) and cubic centimetre (cm^3).
- To convert between different volume units, use these relationships:

  $1\ dm^3 = 1 \times 10^{-3}\ m^3 = 1 \times 10^3\ cm^3 = 1\ L$
- Pressure is the force exerted by a gas on any surface compared to the area of surface. Gases exert pressure on any surface because the constant motion of the particles results in collisions with that surface.
- Pressure is the force exerted on a unit area of a surface.
- The SI unit for pressure is newtons per square metre ($N\ m^{-2}$). In Chemistry, the unit most commonly used is the SI derived unit, the pascal (Pa) or the kilopascal (kPa): $1\ N\ m^{-2} = 1$ Pa and 1 kPa = 1000 Pa.
- The relationship between temperature on the Celsius scale and temperature on the Kelvin scale is given by the equation:

  $T\ (\text{in K}) = T\ (\text{in °C}) + 273$

KEY QUESTIONS

Describe

1 List four physical properties of gases.

2 Define an elastic collision in relation to gases.

3 Define the concept of pressure.

4 True or false: Gases are easy to compress because their particles are in constant motion.

Apply

5 Use the kinetic theory to explain the following observed properties of gases.
- **a** Gases occupy all the available space in a container.
- **b** Gases can be easily compressed compared with their corresponding liquid forms.
- **c** A given volume of a gaseous substance has a mass less than the same volume of the substance in the liquid state.
- **d** Gases mix rapidly.

6 Use the ideas of the kinetic theory of gases to explain the following observations.
- **a** The pressure in a car's tyres will increase if a long distance is travelled on a hot day.
- **b** You can smell dinner cooking from your room.
- **c** A balloon will burst if you blow it up too much.
- **d** Tyre manufacturers state an internal pressure that should not be exceeded.

Analyse

7 Compare the physical properties of gases to those of liquids.

8 Airbags are a safety device fitted to car steering wheels. Determine why a collision with an airbag causes less damage to a driver than a collision with the steering wheel.

9 Pressure is described as the force per unit area of surface. Describe a change to the physical condition of a gas that will increase its pressure. Use kinetic molecular theory to explain this in terms of change to gas particle movement.

10 Predict what will happen to the pressure in each of the following situations using kinetic theory.
- **a** The temperature of a filled aerosol can is increased.
- **b** A gas in a syringe is compressed.

11 Convert the following volumes to the unit specified.
- **a** 2 L to mL
- **b** 3.7 m^3 to L
- **c** 285 mL to m^3
- **d** 100 cm^3 to mL

12 Convert the following temperatures to the unit specified.
- **a** 25°C to K
- **b** 0°C to K
- **b** 300 K to °C
- **c** 373 K to °C

12.2 The ideal gas equation

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- describe the mathematical relationship between pressure, temperature, volume and amount of a gas
- describe the concept of molar volume
- describe the conditions of standard temperature and pressure
- explain the concept of an ideal gas and compare ideal gases to real gases
- state the ideal gas equation ($PV = nRT$) and solve problems using this equation.

The behaviour of gases has been described qualitatively in Module 12.1. In this module, you will learn about the mathematical relationships that link volume, pressure, temperature and the number of particles of a gas.

These mathematical relationships were developed over a period of several hundred years by different scientists who performed experiments on gases. For example, Robert Boyle (Figure 12.2.1) showed by experiment that for a given amount of gas at constant temperature, the volume of the gas is inversely proportional to its pressure. The relationship between gas volume and pressure is known as Boyle's law. Figure 12.2.2 shows Jacques Charles, who identified the relationship between the volume and temperature of a gas. In 1787, Charles determined that the volume of a fixed amount of gas is directly proportional to the absolute temperature, provided the pressure remains constant. The relationship between gas volume and temperature is known as Charles' law.

Relationships like these have become known as the gas laws. The gas laws are used to describe the behaviour of all gases, regardless of their chemical composition.

FIGURE 12.2.1 Robert Boyle (1627–1691) showed by experiment that for a given amount of gas at constant temperature, the volume of a gas is inversely proportional to its pressure.

VOLUME AND PRESSURE

Changing the volume of a fixed amount of gas at constant temperature causes a change in the pressure of the gas. The pressure of the gas in the syringe shown in Figure 12.2.3 increases as the plunger is pushed in and decreases as the plunger is pulled out.

For a given amount of gas at constant temperature, the volume of the gas is inversely proportional to its pressure. This relationship is seen in the changing volume of a weather balloon as it rises to altitudes with much lower pressure than at ground level. A weather balloon filled with helium gas to a volume of 40 L at a pressure of 100 kPa increases in volume to 200 L by the time it reaches an altitude with a pressure of 20 kPa.

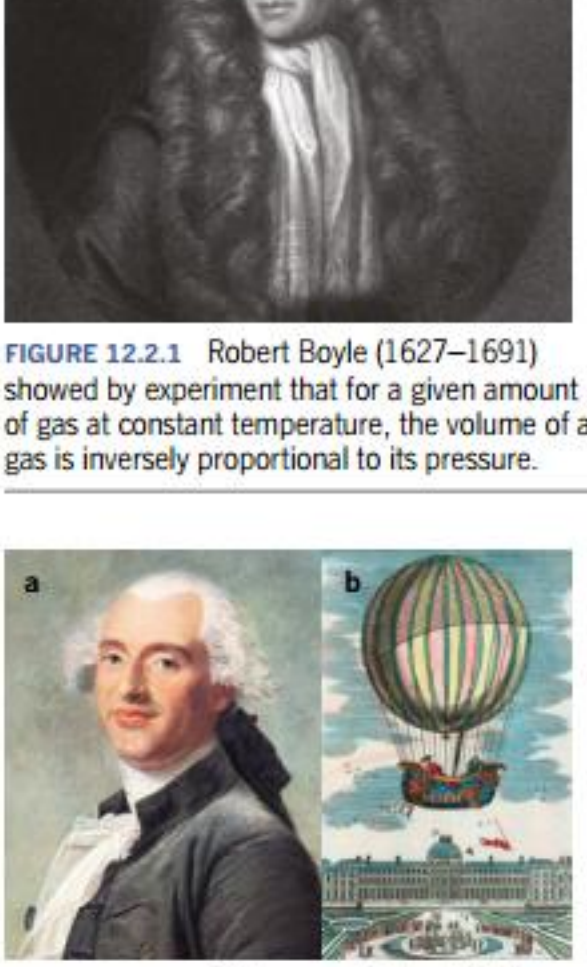


FIGURE 12.2.2 (a) Jacques Charles (1746–1823) identified the relationship between the volume and temperature of a gas. (b) Charles was famous for making the first flight in a hydrogen balloon on 1 December 1783.

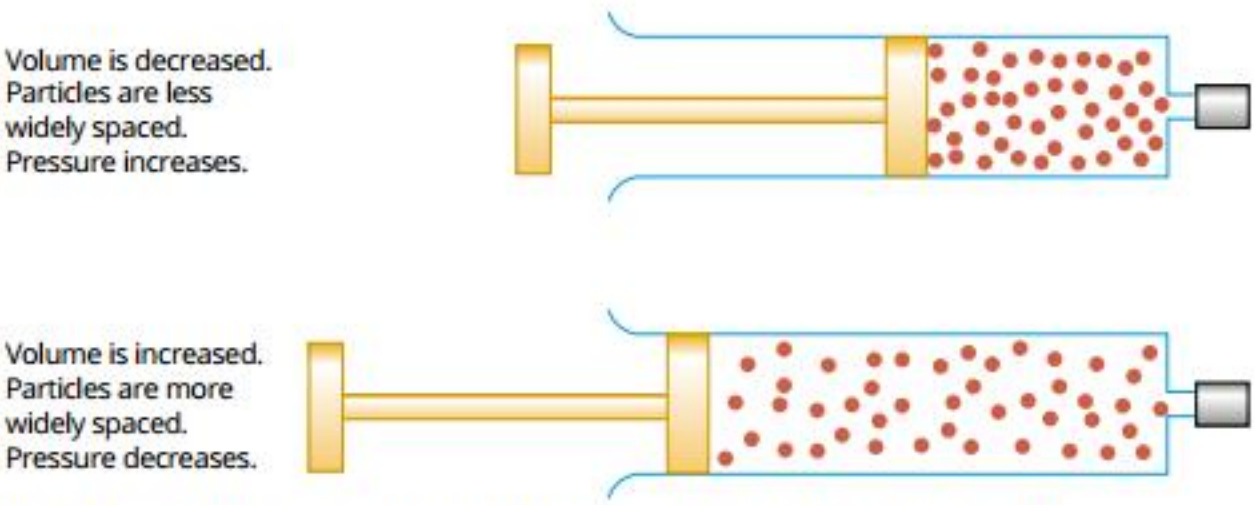


FIGURE 12.2.3 The pressure of the gas in the syringe is affected by a change in volume.

For a fixed amount of gas at a constant temperature, as the pressure increases the volume decreases. The relationship between the volume and pressure of a gas is inversely proportional.

The mathematical relationship between the pressure, P, exerted by a gas and the volume, V, it occupies can be written as:

$$P \propto \frac{1}{V}$$

This relationship can also be expressed as $PV = k$, where k is a constant at a given temperature.

VOLUME AND TEMPERATURE

The kinetic theory states that increasing the temperature of a gas increases the average kinetic energy of the molecules. The molecules move more rapidly and collide with the walls of the container more frequently and with greater force. Increasing the temperature of a gas affects volume and pressure.

- It causes the volume of gas to increase if the pressure on the gas remains the same, such as a gas in a syringe or balloon.
- It causes the pressure to increase if the volume of the gas container is fixed, such as in a sealed flask or a gas cylinder.

The ascending hot-air balloon in Figure 12.2.4 demonstrates the relationship between volume and temperature. Heating the air inside the balloon causes it to expand, which reduces its density and makes it buoyant. This allows the balloon to rise.

FIGURE 12.2.4 Hot air balloonists take advantage of the relationship between the volume of a gas and temperature.

As the temperature, T, of a gas increases, the volume, V, of the gas increases. Therefore, V and T are directly proportional:

$$V \propto T$$

This relationship can also be expressed as $\frac{V}{T} = k$, where k is a constant at a given pressure. Note that the value of T must be expressed in kelvin, not degrees Celsius.

VOLUME AND AMOUNT OF GAS

The volume, V, occupied by a gas also depends directly on the amount of gas, n, in moles. This relationship is shown in Figure 12.2.5. The amount of gas added to the second syringe is double that of the first. If the syringes are both adjusted to the same temperature and pressure, the volume of the gas in the second syringe will be double that of the first.

For a fixed amount of gas at a constant pressure, as the temperature increases the volume increases. The relationship between the volume and temperature of a gas is directly proportional.

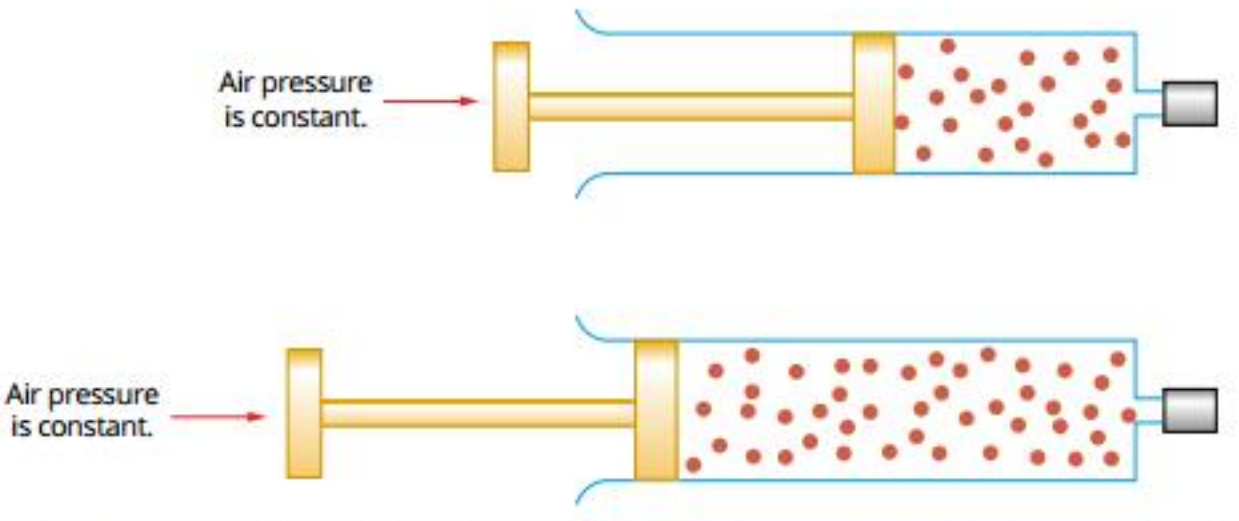


FIGURE 12.2.5 When the amount of gas in the syringe is doubled, the volume doubles, provided the pressure on the plunger and the temperature of the gas remain constant.

The relationship between the number of moles and volume of gas is directly proportional. If pressure and temperature are constant, as the moles of gas increase the volume increases.

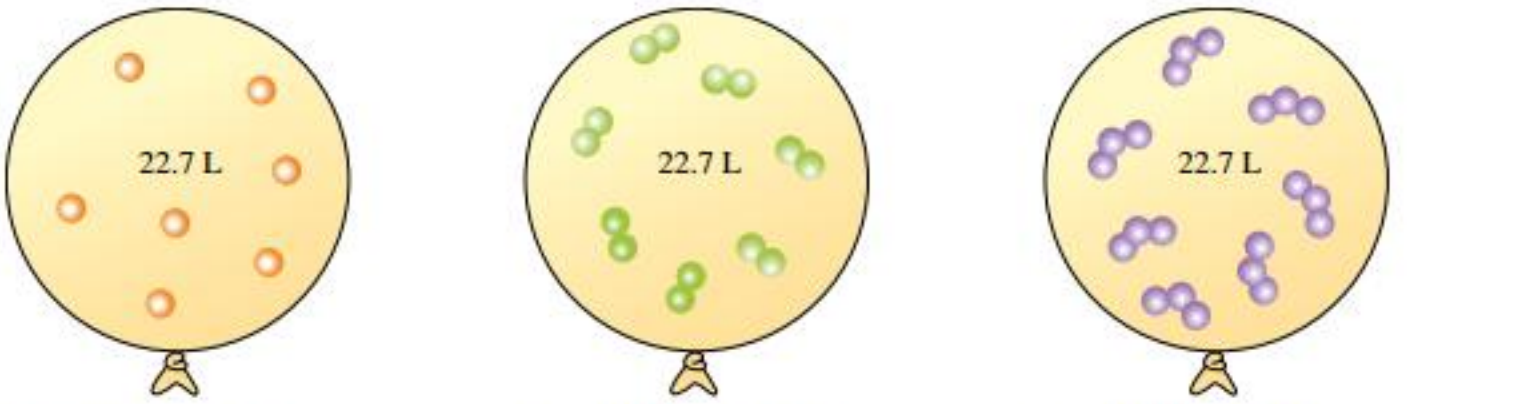
The mathematical relationship between the volume, V, occupied by a gas and the amount in moles of gas, n, at constant temperature and pressure can be written as:

$$V \propto n$$

This relationship can also be expressed as $\frac{V}{n} = k$, where k is a constant at a given temperature and pressure.

Molar volume

If the amount of gas is fixed at 1 mole as shown in Figure 12.2.6, the volume it occupies depends almost entirely on its temperature and pressure. This volume is defined as the **molar volume**, V_m, of a gas. Molar volume is the amount of space, or volume, occupied by 1 mole of any gas at a particular pressure and temperature.



1 mole of neon, Ne
$P = 100$ kPa
$T = 0°C$
$V = 22.7$ L
number of molecules = 6.02×10^{23}
mass = 20.18 g

1 mole of nitrogen, N_2
$P = 100$ kPa
$T = 0°C$
$V = 22.7$ L
number of molecules = 6.02×10^{23}
mass = 28.02 g

1 mole of ozone, O_3
$P = 100$ kPa
$T = 0°C$
$V = 22.7$ L
number of molecules = 6.02×10^{23}
mass = 48.00 g

FIGURE 12.2.6 One mole of any gas occupies the same volume given the same temperature and pressure.

The volume of 1 mole of gas, V_m, is equal to its total volume, V, divided by the number of moles, n, of gas present. This can be represented by the relationship:

$$V_m = \frac{V}{n} \text{ (at a given temperature and pressure)}$$

Or, by rearranging this expression:

$$n = \frac{V}{V_m} \text{ (at a given temperature and pressure)}$$

The molar volume of a gas varies with temperature and pressure. However, molar volume does not vary with the identity of the gas. For example, 1 mole of hydrogen gas occupies the same volume as 1 mole of oxygen gas at the same temperature and pressure.

Standard temperature and pressure

A commonly used set of standard conditions is **standard temperature and pressure (STP)**. STP refers to a temperature of 0°C (273 K) and a pressure of 100 kPa. The molar volume of any gas at STP is 22.7 L mol^{-1}.

$V_m = 22.7$ L mol^{-1} (or dm^3 mol^{-1}) at STP (0°C or 273 K and 100 kPa)

Worked example 12.2.1

CALCULATING THE VOLUME OF A GAS FROM ITS NUMBER OF MOLES AT STP

Calculate the volume, in L, occupied by 0.24 mol of nitrogen gas at STP.	
Thinking	**Working**
Rearrange $n = \frac{V}{V_m}$ to make volume the subject.	$n = \frac{V}{V_m}$ $V = n \times V_m$
Substitute in the known values where V_m = 22.7 L mol^{-1} (at STP) and solve.	$V = n \times V_m$ $= 0.24 \times 22.7$ $= 5.448$ L
Consider the units and significant figures. The answer should be given to the smallest number of significant figures in the measurement.	$V = 5.4$ L

➤ Try yourself 12.2.1

CALCULATING THE VOLUME OF A GAS FROM ITS NUMBER OF MOLES AT STP

Calculate the volume, in L, occupied by 3.5 mol of oxygen gas at STP.

IDEAL GASES

An **ideal gas** is one that obeys the gas laws exactly, at all conditions of temperature and pressure. It is a hypothetical gas whose molecules occupy negligible space and have no interactions with other particles. Gases that exist in the real world come very close to ideal gas behaviour, but under conditions of very low temperature or very high pressure, these laws no longer apply exactly. A gas like this is called a **real gas**. We can assume that a gas at standard temperature and pressure will follow ideal gas behaviour.

As you have seen, the following three laws describe the behaviour of gases under different conditions:

- $V \propto \frac{1}{V}$ (for constant T and n)
- $V \propto T$ (for constant P and n)
- $V \propto n$ (for constant P and T).

All three laws can be combined by writing:

$$V \propto \frac{nT}{P}$$

This relationship can be expressed as $V = \frac{RnT}{P}$, where R is a proportionality constant. The equation is known as the **ideal gas equation** and is more usually written in the form:

$$PV = nRT$$

where R is called the ideal gas constant, or simply the **gas constant**.

This constant can be determined experimentally by measuring the volume occupied by a known amount of gas at a known temperature and pressure. The value of R depends on the units of pressure and volume used. It has a value of 8.31 JK^{-1} mol^{-1} when:

- P is measured in kilopascals, kPa
- V is measured in litres, L
- n is measured in moles, mol
- T is measured in kelvin, K.

Worked example 12.2.2

CALCULATING THE VOLUME OF A GAS USING THE IDEAL GAS EQUATION

Calculate the volume, in L, occupied by 2.24 mol of oxygen gas (O_2) if the pressure is 200.0 kPa at 50.0°C.

Thinking	Working
Convert units, if necessary. Pressure is in kPa and temperature in K.	$P = 200.0\,\text{kPa}$ (no conversion required) $T = 50.0 + 273$ $= 323\,\text{K}$
Rearrange the ideal gas equation so that volume, V, is the subject.	$PV = nRT$ $V = \frac{nRT}{P}$
Substitute values for pressure, amount, temperature and the gas constant, R, then solve for V. Express the answer to the correct number of significant figures.	$V = \frac{2.24 \times 8.31 \times 323}{200.0}$ $= 30.1\,\text{L}$

➤ Try yourself 12.2.2

CALCULATING THE VOLUME OF A GAS USING THE IDEAL GAS EQUATION

Calculate the volume, in L, occupied by 13.0 mol of carbon dioxide gas (CO_2) if the pressure is 250 kPa at 75.0°C.

12.2 Review

SUMMARY

- For a given amount of gas at constant temperature, the volume of the gas is inversely proportional to its pressure.

  $P \propto \frac{1}{V}$
- For a given amount of gas at constant pressure, the volume of the gas is directly proportional to its temperature. $V \propto T$
- For a gas at constant pressure, the volume of the gas is directly proportional to the amount of gas in moles. $V \propto n$
- Molar volume (V_m) is the amount of space, or volume, occupied by 1 mole of any gas at a particular pressure and temperature.
- Standard temperature and pressure (STP) refers to a temperature of 0°C (273 K) and a pressure of 100 kPa.
- The value of V_m at STP is $22.7\,\text{L mol}^{-1}$.
- An ideal gas is a hypothetical gas whose molecules occupy negligible space and have no interactions, and which consequently obeys the gas laws exactly.
- Gases that exist in the real world are called real gases. Real gases obey the gas laws except at very high pressures and very low temperatures.
- $PV = nRT$ is the ideal gas equation. It can be used to calculate one variable (P, V, n or T) when the other three variables are known.
- R is the ideal gas constant and its value is $8.31\,\text{J K}^{-1}\,\text{mol}^{-1}$ when pressure is in kPa, volume is in L, amount is in mol and temperature is in K.

12.2 Review *continued*

KEY QUESTIONS

Describe

1 Describe the relationship between the volume and pressure of a gas, assuming temperature is constant.

2 Describe the mathematical relationship between temperature and volume, assuming pressure is constant.

3 What does the term 'molar volume' mean?

4 Define the term 'ideal gas'.

5 Identify if this statement is true or false. In the ideal gas equation, the value of R is independent of the units of pressure and volume used. It always has a value of $8.31\,J\,K^{-1}\,mol^{-1}$.

6 State the ideal gas equation, and the units that must be used when calculating values using this equation.

Apply

7 When the gas inside a syringe is compressed, the volume decreases and the pressure increases. Explain why.

8 Explain, using your understanding of the relationship between the temperature and volume of gases, how a hot air balloon floats.

9 Use your understanding of the relationship between temperature and pressure of gases to explain why a party balloon might pop when brought into a hot room.

10 The molar volume of a gas varies with temperature and pressure. Explain why the molar volume of a gas does not vary with the identity of the gas.

Analyse

11 When a weather balloon rises in the atmosphere, its volume increases. However, at higher altitudes there is a drop in temperature. Suggest a reason why the balloon does not decrease in volume.

12 Under what conditions might a gas not obey the rules of the kinetic molecular theory, and no longer be described as an ideal gas?

13 Calculate the volume of the following gases at STP.

a 1.4 moles of chlorine (Cl_2)

b 1.0×10^{-3} moles of hydrogen (H_2)

c 1.4 g of nitrogen (N_2)

14 Calculate the mass of the following gas samples. All volumes are measured at STP.

a 2.80 L of neon (Ne)

b 50.0 L of oxygen (O_2)

c 140 mL of carbon dioxide (CO_2)

15 0.263 mol of a gas occupies 9.0 L at a certain temperature and pressure. Calculate its molar volume at this temperature and pressure.

16 A flask of volume 5.0 L at a temperature of 5°C contains 0.25 moles of nitrogen. Determine the pressure in the flask.

17 Calculate the volume of gas, in litres, occupied by:

a 0.20 moles of hydrogen at 115 kPa and 40°C

b 12.5 moles of carbon dioxide at 507 kPa and 150°C

c 8.50 g of hydrogen sulfide (H_2S) at 100 kPa and 27°C.

18 Calculate the mass of helium in a balloon if the volume is 100 L at a pressure of 95 000 Pa and a temperature of 0°C.

19 At a given temperature, a sample of nitrogen, of mass 11.3 g, exerts a pressure of 102 kPa in a gas cylinder of volume 10.0 L. Calculate the temperature of the gas.

20 Which sample of gas contains the greater amount in moles: 3.2 L of nitrogen at 25°C and a pressure of 120 kPa or 2.5 L of helium at 23°C and a pressure of 122 kPa?

21 A student experimentally determined that 1.482 g of a gas occupied a volume of 16.8 L at STP. Calculate the molar mass of the gas, and thus determine its identity.

12.3 Gas stoichiometry

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- use stoichiometry to perform mass–volume calculations
- use stoichiometry to perform volume–volume calculations
- determine the excess reagent for reactions involving gases.

In Chapter 9, you learnt that stoichiometric calculations allow you to use the mole ratio to predict the amount of product that will be formed or how much reactant will be used. Measuring and predicting quantities is a very important part of chemistry. For example, scientists can compare fuels by calculating the quantities of chemicals involved in their reactions. The combustion of ethanol can be compared to the combustion of petroleum by calculating how much oxygen is required for complete combustion. This allows the amount of atmospheric pollution a fuel will produce to be determined by calculating the mass of carbon dioxide given off (Figure 12.3.1).

In this module, you will apply stoichiometry to chemical reactions involving gases.

FIGURE 12.3.1 It is useful to be able to calculate the volume of carbon dioxide emissions produced by the combustion of a particular fuel.

STOICHIOMETRY INVOLVING GASES

As you learnt in Chapter 9, calculations that involve the use of the mole concept, combined with an understanding of chemical equations, are called stoichiometric calculations.

The steps and details of formulas used when performing stoichiometric calculations involving gases are summarised in Figure 12.3.2.

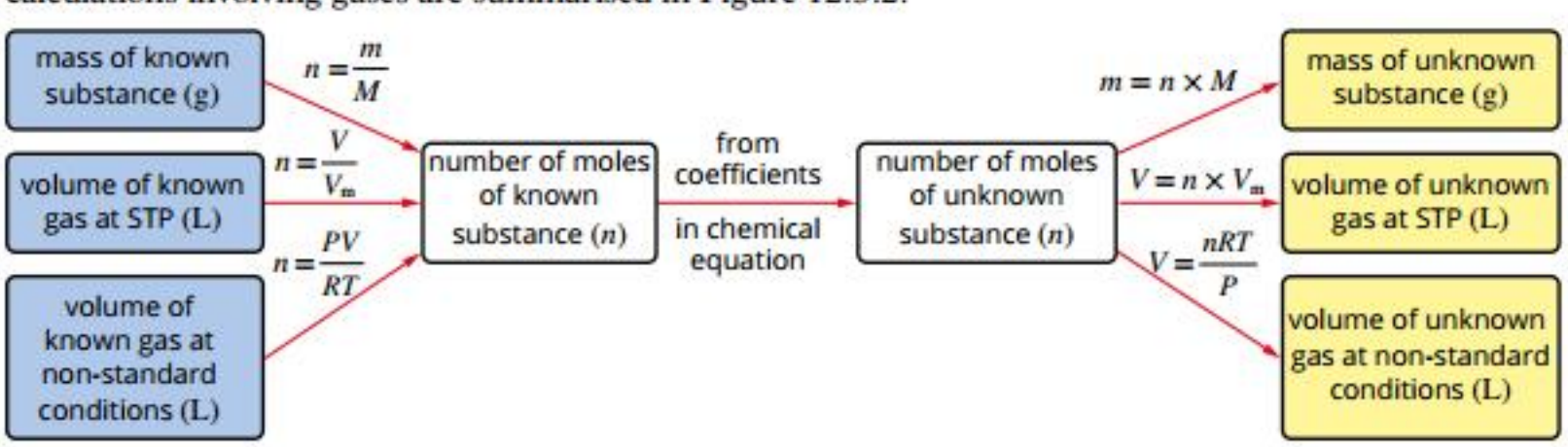

mass of known substance (g)
volume of known gas at STP (L)
volume of known gas at non-standard conditions (L)
$n = \frac{m}{M}$
$n = \frac{V}{V_m}$
$n = \frac{PV}{RT}$
number of moles of known substance (n)
from coefficients in chemical equation
number of moles of unknown substance (n)
$m = n \times M$
$V = n \times V_m$
$V = \frac{nRT}{P}$
mass of unknown substance (g)
volume of unknown gas at STP (L)
volume of unknown gas at non-standard conditions (L)

FIGURE 12.3.2 Most stoichiometric calculations follow the steps shown in the flow chart. Calculating the number of moles and using a mole ratio from a balanced chemical equation are always central to any stoichiometric calculation.

Mass–volume stoichiometry

Some stoichiometric calculations require you to determine the volume of a gas produced from a given mass of reactant. For these calculations, you need to determine the number of moles of the reactant using its mass, and to use the mole ratio from the balanced chemical equation.

The volume of the gas, in litres, is determined from its number of moles using the formula:

1 At STP (0°C and 100 kPa), the molar volume equation is used:

$$n = \frac{V}{V_m}$$

This formula can be rearranged to make volume the subject:

$$V = n \times V_m$$

Remember that at STP, the accepted volume of 1 mole of any gas is 22.7 L mol^{-1}.

2 At non-standard conditions, the ideal gas equation is used:

$$PV = nRT$$

The ideal gas equation can also be rearranged to make volume the subject:

$$V = \frac{nRT}{P}$$

Remember that for use in the ideal gas equation, pressure must be in kPa, temperature must be in K and the gas constant is equal to $8.31\,J\,K^{-1}\,mol^{-1}$.

Worked example 12.3.1

MASS–VOLUME STOICHIOMETRIC CALCULATIONS AT STANDARD TEMPERATURE AND PRESSURE (STP)

Calculate the volume of carbon dioxide, in L, produced when 2.00 kg of propane is burnt completely in oxygen. The gas volume is measured at STP.	
Thinking	**Working**
Write a balanced equation for the reaction.	$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$
Molar mass of propane (C_3H_8) = 44.11 g Calculate the number of moles of the known substance using: $n = \frac{m}{M}$	$n(C_3H_8) = \frac{2000}{44.11}$ $= 45.3\,mol$
From the balanced equation determine the mole ratio of carbon dioxide formed from propane burnt: $\text{mole ratio} = \frac{\text{coefficient of unknown}}{\text{coefficient of known}}$	$\frac{\text{coefficient of } CO_2}{\text{coefficient of } C_3H_8} = \frac{3}{1}$
Calculate the number of moles of the unknown substance using: $n(\text{unknown}) = \text{mole ratio} \times n(\text{known})$	$n(CO_2) = \frac{3}{1} \times 45.3$ $= 135.9\,mol$
Calculate the volume of the unknown substance using: $V = n \times V_m$	$V(CO_2) = 135.9 \times 22.7$ $= 3084.93\,L$ $= 3.08 \times 10^3\,L$

➤ Try yourself 12.3.1

MASS–VOLUME STOICHIOMETRIC CALCULATIONS AT STANDARD TEMPERATURE AND PRESSURE (STP)

Calculate the volume of carbon dioxide, in L, produced when 300 g of butane is burnt completely in oxygen. The gas volume is measured at STP.

Worked example 12.3.2

MASS–VOLUME STOICHIOMETRIC CALCULATIONS AT NON-STANDARD CONDITIONS

Calculate the volume of carbon dioxide, in L, produced when 800 g of propane is burnt completely in oxygen. The gas volume is measured at 60°C and 200 kPa.	
Thinking	**Working**
Write a balanced equation for the reaction.	$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$

Calculate the number of moles of the known substance using: $n = \frac{m}{M}$	$n(C_3H_8) = \frac{800}{44.11}$ $= 18.1\,\text{mol}$
From the balanced equation determine the mole ratio of carbon dioxide formed from propane burnt: $\text{mole ratio} = \frac{\text{coefficient of unknown}}{\text{coefficient of known}}$	$\frac{\text{coefficient of } CO_2}{\text{coefficient of } C_3H_8} = \frac{3}{1}$
Calculate the number of moles of the unknown substance using: $n(\text{unknown}) = \text{mole ratio} \times n(\text{known})$	$n(CO_2) = \frac{3}{1} \times 18.1$ $= 54.3\,\text{mol}$
Express the pressure and temperature in required units.	$P = 200\,\text{kPa}$ $T = 60 + 273 = 333\,\text{K}$
Calculate the volume of the unknown substance using: $V = \frac{nRT}{P}$	$V(CO_2) = \frac{54.3 \times 8.31 \times 333}{200} = 751\,\text{L}$

➤ **Try yourself 12.3.2**

MASS–VOLUME STOICHIOMETRIC CALCULATIONS AT NON-STANDARD CONDITIONS

Calculate the volume of carbon dioxide, in L, produced when 5.00 kg of butane is burnt completely in oxygen. The gas volume is measured at 40°C and 400 kPa.

Volume–volume stoichiometry

For chemical reactions in which both the reactants and products are in the gaseous state, it is often convenient to measure volumes, rather than masses. For example, the reaction between propane gas and oxygen can be represented by the equation:

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$$

This equation tells us that when 1 mole of propane gas reacts with 5 moles of oxygen gas, 3 moles of carbon dioxide gas and 4 moles of water vapour are produced.

You saw in Module 12.2 that if gases are behaving in an ideal way, the molar volume of any gas is the same. Therefore, the mole ratios in the balanced equation become volume ratios at the same temperature and pressure. In the above reaction, this means that when 1 litre of propane gas reacts with 5 litres of oxygen gas, 3 litres of carbon dioxide gas and 4 litres of water vapour are produced.

Worked example 12.3.3

GAS VOLUME–VOLUME CALCULATIONS

Methane gas (CH_4) is burnt in a gas stove according to the following equation:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$$

If 50 mL of methane is burnt, calculate the volume of O_2 gas required for complete combustion of the methane under constant temperature and pressure conditions.

Thinking	Working
Use the balanced equation to find the mole ratio of the two gases involved.	1 mole of CH_4 gas reacts with 2 moles of O_2 gas.
The temperature and pressure are constant, so volume ratios are the same as mole ratios.	1 volume of CH_4 reacts with 2 volumes of O_2 gas, so 50 mL of CH_4 reacts with 100 mL of O_2.

➤ Try yourself 12.3.3

GAS VOLUME–VOLUME CALCULATIONS

Methane gas (CH_4) is burnt in a gas stove according to the following equation:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$$

If 50 mL of methane is burnt in air, calculate the volume of CO_2 gas produced under constant temperature and pressure conditions.

Calculations involving excess reactants

As you learnt in Chapter 9, stoichiometry calculations become more complex if the reactants are not present in their stoichiometric ratio. In these cases, you must determine which reactant is completely consumed in the reaction, the limiting reactant, and which one is present in excess. The amount of limiting reactant determines how much product is formed.

Worked example 12.3.4 introduces a strategy that can be used to determine the limiting reactant in a reaction.

Worked example 12.3.4

EXCESS REACTANT CALCULATIONS

A gaseous mixture of 25.0 g of hydrogen gas and 100.0 g of oxygen gas is ignited. The water produced is collected and weighed. Calculate the theoretical mass of water produced. The equation for the reaction is:

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$

a Determine which reactant is the limiting reactant.

b Calculate the mass of water vapour formed.

Thinking	Working
a Calculate the number of moles of each reactant using $n = \frac{m}{M}$ or $n = \frac{V}{V_m}$ as appropriate.	$n(H_2) = \frac{m}{M}$ $= \frac{25.0}{2.02}$ $= 12.4\,\text{mol}$ $n(O_2) = \frac{m}{M}$ $= \frac{100.0}{32.00}$ $= 3.13\,\text{mol}$
Use the coefficients of the equation to determine the limiting reactant.	The equation shows 2 moles of H_2 reacts with 1 mole of O_2. So to react all of the O_2 will require: $2 \times n(O_2)$ of H_2 $= 2 \times 3.13$ $= 6.26\,\text{mol}$ As there are 12.4 moles of H_2, the H_2 is in excess. The O_2 is the limiting reactant (it will be completely consumed).
b Determine the mole ratio using: $\frac{\text{coefficient of unknown}}{\text{coefficient of known}}$ The limiting reactant is the known substance.	$\frac{n(H_2O)}{n(O_2)} = \frac{2}{1}$

Calculate the number of moles of the unknown substance using: n(unknown) = mole ratio × n(known)	$n(H_2O) = 2 \times 3.13$ $= 6.26$ moles
Calculate the required quantity of the unknown using $m = n \times M$ or $n = \frac{V}{V_m}$ or $PV = nRT$ as appropriate.	$m(H_2O) = 6.26 \times 18.02$ $= 113$ g

➤ Try yourself 12.3.4

EXCESS REACTANT CALCULATIONS

Calculate the volume of carbon dioxide, in L, produced when 65.0 g of butane is burnt completely in 200 L of oxygen. The gas volume is measured at STP. The equation for the reaction is:

$$2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(l)$$

a Determine which reactant is the limiting reactant.

b Calculate the volume of carbon dioxide formed.

12.3 Review

SUMMARY

- Stoichiometry is the study of ratios of the amount of moles of substances reacted or produced in a chemical reaction.
- A balanced equation shows the ratio of the amount, in moles, of reactants and products in the reaction.
- Stoichiometric calculations follow these general steps.
  1 Calculate the number of moles of a known substance from the data given.
  Use $n = \frac{m}{M}$, $n = \frac{V}{V_m}$ or $n = \frac{PV}{RT}$.
  2 Use the mole ratio from a balanced chemical equation to determine the amount, in moles, of the unknown substance.
  3 Find the desired quantity of the unknown substance from its amount, in moles, using:
  $m = n \times M$, $V = n \times V_m$ or $PV = nRT$

KEY QUESTIONS

Describe

1 Define 'stoichiometry'.

Apply

2 Summarise the steps to follow when solving mass–volume stoichiometric calculations.

3 Why it is possible to use mole ratios in the balanced equation as volume ratios?

4 Provide formulas for two different ways the amount of a gas can be calculated from a given volume. Explain when you should use each formula.

Analyse

5 Propane (C_3H_8) burns in oxygen according to the equation:

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$

When the following masses of propane react completely with excess oxygen, calculate the volume of:

i oxygen used at STP

ii carbon dioxide produced at STP

a 22 g

b 3.40 kg

6 Octane is one of the main constituents of petrol. It burns according to the equation:

$$2C_8H_{18}(g) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(g)$$

Calculate the mass of octane that must have been used if 50.0 L of carbon dioxide, measured at 120°C and 111 kPa, was produced.

7 Hydrogen peroxide decomposes according to the equation:

$$2H_2O_2(aq) \rightarrow 2H_2O(l) + O_2(g)$$

Calculate the volume of oxygen, collected at 30.0°C and 91.0 kPa, that is produced when 10.0 g of hydrogen peroxide decomposes.

8 Determine the volume of NO_2 produced when 0.5 L of nitrogen(II) oxide (NO) reacts with excess oxygen. (All volumes are measured at 25°C and 100 kPa.)
The equation for the reaction is:

$$2NO(g) + O_2(g) \rightarrow 2NO_2(g)$$

9 Calculate the volume of oxygen needed to completely react with 150 mL of carbon monoxide according to the following equation. Assume all volumes are measured at the same temperature and pressure.

$$2CO(g) + O_2(g) \rightarrow 2CO_2(g)$$

10 Calculate the pressure produced in a sealed 100.0 mL container, when 1.00 g of liquid water is vapourised at 220.0°C.

11 15.0 g of methane gas is reacted with 10.0 L of oxygen at STP. Calculate the volume of carbon dioxide at STP produced in this reaction. The equation for this reaction is:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$$

12 A 1.52 g piece of aluminium metal reacts completely with a solution of sulfuric acid to produce aqueous aluminium sulfate and hydrogen gas:

$$2Al(s) + 3H_2SO_4(aq) \rightarrow Al_2(SO_4)_3(aq) + 3H_2(g)$$

a Calculate the mass of hydrogen produced.

b Determine the volume of hydrogen gas produced at STP.

Chapter review

12

KEY TERMS

density
elastic collision
gas constant
ideal gas
ideal gas equation
intermolecular force
Kelvin scale
kilopascal
kinetic energy
kinetic theory
molar volume
pascal
pressure
real gas
standard temperature and pressure (STP)
stoichiometry
volume

KEY QUESTIONS

Describe

1 Identify which of the following volumes is equal to 4.5 L.
- **A** 4.5×10^{-3} mL
- **B** 4.5×10 mL
- **C** 4.5×10^{2} mL
- **D** 4.5×10^{3} mL

2 Identify which one of the following statements best describes the effect of an increase in temperature on gas particles.
- **A** Both the average kinetic energy and the average speed of the particles increase.
- **B** Both the average kinetic energy and the average speed of the particles decrease.
- **C** The average kinetic energy of the particles decreases and the average speed of the particles increases.
- **D** The average kinetic energy of the particles increases and the average speed of the particles decreases.

3 Select the correct answers from the pairs of words to complete the paragraph about gases.
The volume occupied by the atoms or molecules in a gas is much *smaller/larger* than the total volume occupied by the gas. The particles move in rapid, *straight-line/curved* paths and collide with each other and with the walls of the container. The forces between particles are extremely *weak/strong*. The collisions between particles are *elastic/rigid*. The average kinetic energy of the particles is *directly/inversely* proportional to the temperature of the gas, in units of *K/°C*.

4 State the ideal gas equation.

5 State the value of the gas constant, *R*, assuming pressure is measured in kPa, volume in L, and temperature in K.

6 State the name of the law that stoichiometric calculations are based on.

Apply

7 Use the kinetic theory of gases to explain the following.
- **a** The pressure of a gas increases if its volume is reduced at constant temperature.
- **b** The pressure of a gas decreases if its temperature is lowered at a constant volume.
- **c** In a mixture of gases, the total pressure is the sum of the partial pressure of each gas.
- **d** The pressure of a gas, held at constant volume and temperature, will increase if more gas is added to the container.

8 Explain how the relationship between the temperature and volume of gases led to the development of the Kelvin scale.

9 Most gases, under most conditions, behave in an ideal way. Explain under what circumstances gases tend not to follow the gas laws.

Analyse

10 A weather balloon filled with helium gas has a volume of 20 L at 100 kPa. After being released, it rises into the atmosphere where it reaches an altitude with a pressure of 20 kPa. The balloon increases in volume to 100 L. Explain why this occurs in terms of the relationship between the pressure and volume of gases.

11 Consider two containers of equal size; one contains oxygen and the other carbon dioxide. Both containers are at 18°C and at a pressure of 100 kPa. Answer the following questions about the two gas samples, and give a reason for your answers.
- **a** Does one container have more molecules than the other and, if so, which one?
- **b** Which of the two samples contains the greater number of atoms?
- **c** Density is defined as the mass per unit volume $\left(\frac{m}{V}\right)$. Is the density of both gases the same? If not, which has the greater density?

12 The molar volume of a gas varies with temperature and pressure. However, molar volume does not vary with the identity of the gas. Consider and explain why this is the case.

13 Convert the following values to the units specified.
- **a** 1.7 L to mL
- **b** 203 000 Pa to kPa
- **c** 57 K to °C

14 Calculate the mass of oxygen (O_2) present in a 50.0 L container of oxygen at STP.

15 If 64.0 g of oxygen gas occupies a volume of 25.0 L when the temperature is 303 K, then the pressure of the gas, in kPa, is closest to:
- **A** 20.0
- **B** 200
- **C** 400
- **D** 6.4×10^3

16 Use the molar volume of a gas at STP to determine the:
- **a** volume occupied by 8.0 g of oxygen at STP
- **b** mass of nitrogen dioxide present in 10.0 L at STP

17 Calculate the volume, in litres, occupied by 10.0 g of carbon dioxide at 25°C and 100 kPa.

18 Determine the mass of oxygen present in a 10.0 L container of oxygen at a pressure of 105 kPa and at 20°C.

19 Calculate the temperature required for 0.2 g of helium to exert a pressure of 80 kPa in a container with a fixed volume of 4.0 L.

20 A sample of gas of mass 10.0 g occupies a volume of 5.4 L at 27°C and 100×10^3 Pa.
- **a** Calculate the number of moles of gas in the sample.
- **b** Determine the molar mass of the gas.

21 Determine which container holds more molecules of oxygen gas: container A of volume 40.0 L at 25°C and 103 kPa or container B of volume 0.10 L at 45°C and 52 kPa.

22 A room has a volume of 220 m^3.
- **a** Calculate the number of moles of air particles in the room at 23°C and a pressure of 100 kPa.
- **b** Assume that 20% of the molecules in the air are oxygen molecules and the remaining molecules are nitrogen. Calculate the mass of air in the room.

23 Octane is one of the main constituents of petrol. It burns according to the equation:

$$2C_8H_{18}(g) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(g)$$

Calculate the mass of octane used if 16.3 L of carbon dioxide, measured at 105°C and 101.3 kPa, was produced.

24 Large quantities of coal are burned in Australia to generate electricity. This also generates significant amounts of the greenhouse gas $CO_2(g)$. The equation for this reaction is:

$$C(s) + O_2(g) \rightarrow CO_2(g)$$

Determine the mass of carbon dioxide produced by the combustion of 1.0 tonne (10^6 g) of coal. (Assume that the coal is pure carbon.)

25 Calculate the volume of oxygen gas (in L) required for the complete combustion of 10.0 L of ethane gas at constant pressure and a temperature of 150°C.

26 Methane burns in excess oxygen according to the equation:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$$

This reaction produces 5 L of carbon dioxide at 200°C and 100 kPa. Assuming all volumes are measured at the same temperature and pressure, calculate the:
- **a** volume of methane used
- **b** volume of oxygen used
- **c** mass of water vapour produced

Interpret

27 A sample of gas of mass 9.604 g occupies a volume of 5.44 L at 27°C and 100×10^3 Pa.
- **a** Calculate the amount, in mol, of gas in the sample.
- **b** Use this to determine the molar mass of the gas.
- **c** Suggest a possible identity of the gas.

28 Propane undergoes complete combustion as follows:

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$$

All volumes are measured at 120°C and 100 kPa. An 80 mL volume of propane and 500 mL of oxygen are reacted.
- **a** One of the gases does not react completely. Determine which gas is in excess and calculate the volume that is unreacted.
- **b** Calculate the volumes of carbon dioxide and water that are produced in the reaction.
- **c** Calculate the change in total volume of all the gases that has occurred as a result of the reaction.

29 An indoor gas heater burns propane (C_3H_8) at a rate of 12.7 g per minute. Determine the minimum mass of oxygen per minute, in g, that needs to be available for the complete combustion of propane.

30 The Gladstone Power Station, Queensland's largest, consumes about 4.0 million tonnes (1 tonne = 10^6 g) of coal in one year. The coal used in the power station is composed of approximately 25% carbon. Determine the volume of the greenhouse gas carbon dioxide released each year by the power station at STP.

31 Scientists around the world are investigating possible replacements for fossil fuels. A group of Japanese chemists is investigating the following reaction as a source of methane for fuel:

$$CaCO_3(s) + 4H_2(g) \rightarrow CH_4(g) + Ca(OH)_2(s) + H_2O(g)$$

If the reaction is conducted at 400°C and 100 kPa, calculate the:
- **a** volume of methane produced if 100 L of hydrogen gas is completely reacted.
- **b** mass of calcium carbonate required in part a.

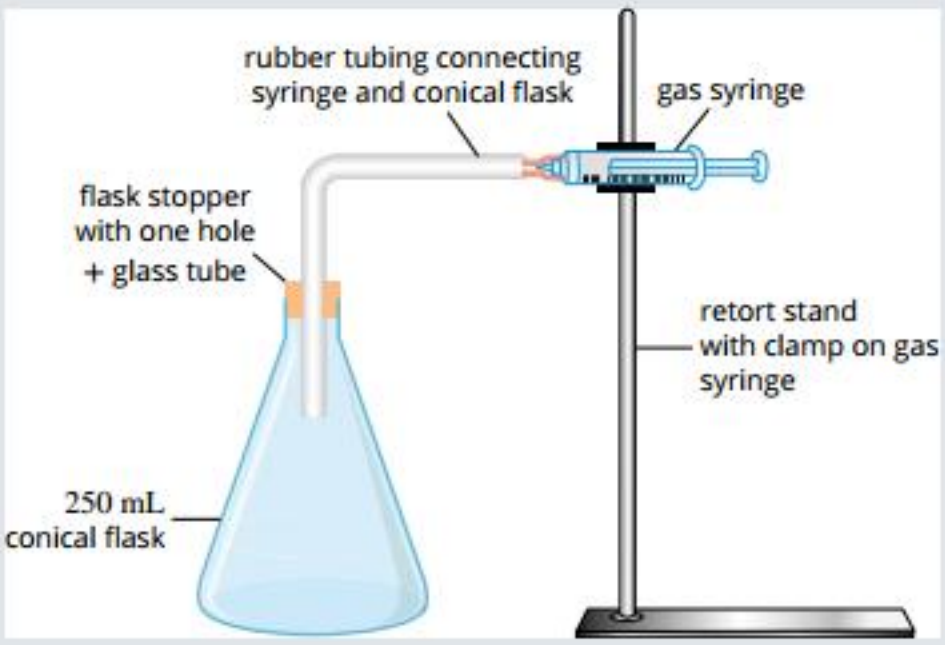
Data analysis

DATA SET 1

The information below applies to Questions 1–4.

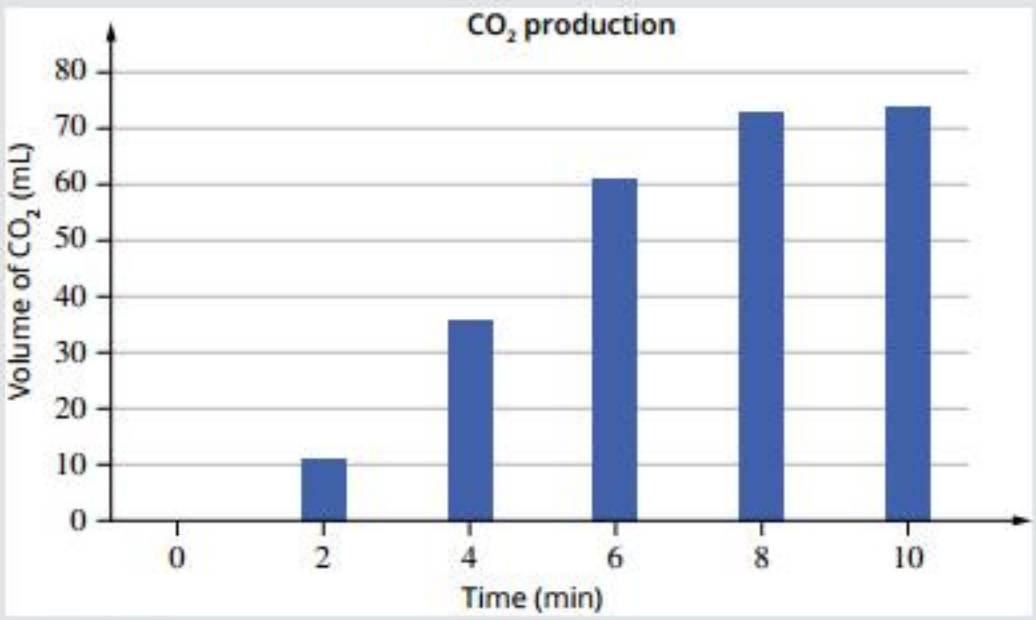
An experiment is carried out where sodium carbonate is reacted with hydrochloric acid according to the balanced chemical equation. The experimental setup is shown below. 0.004 mole of sodium carbonate was added to excess HCl in the flask and the stopper immediately replaced. Assume standard temperature and pressure.

$$Na_2CO_3(s) + 2HCl(aq) \rightarrow 2NaCl(aq) + CO_2(g) + H_2O(l)$$


rubber tubing connecting syringe and conical flask
gas syringe
flask stopper with one hole + glass tube
retort stand with clamp on gas syringe
250 mL conical flask

Experimental data is tabulated and graphed below.

Time (min)	Volume CO_2 (mL) at STP
0	0
2	11.00
4	36.00
6	61.00
8	73.00
10	74.00



Question 1 (1 mark)

Identify the volume of CO_2 produced.

Question 2 (2 marks)

Using the experimental data, calculate the molar volume of CO_2.

Question 3 (3 marks)

Contrast your experimental value with the known molar gas volume (at STP), calculate the percentage error of the experimental value and provide a possible reason for this lack of accuracy.

Question 4 (3 marks)

The experiment was repeated in a different laboratory and different city. 100 mL of CO_2 gas was collected. The altitude of the new laboratory is higher than original laboratory, leading to an atmospheric pressure decrease of 5%. Deduce the temperature of this new laboratory. Provide your answer in °C.

CHAPTER

13 Water and aqueous solutions

The water you see and use every day is a unique chemical with unusual properties. In this chapter, you will learn about some of the unusual properties of water and how they can be explained by the intermolecular bonds that water can form with itself and with other compounds. You will investigate how these intermolecular forces increase its melting and boiling points. Learning about properties such as latent heat and density will enable you to understand the role water plays in biological and environmental systems.

Water is often described as the universal solvent because it can dissolve a wide range of substances. The Earth's oceans, rivers and lakes are aqueous solutions containing many different dissolved minerals and gases. The plasma of human blood and the sap of plants are aqueous solutions carrying dissolved nutrients and wastes. In this chapter, you will learn how different types of substances dissolve in water and how to predict whether a compound is likely to be soluble or insoluble in water. The polarity of water plays a critical role in determining the compounds that can be dissolved in it.

Solubility is the term used to describe how much of a compound will dissolve in a particular amount of water. You will learn how to determine how much of a substance will dissolve in a given amount of water at a particular temperature. You will also look at the different units used by chemists to measure the concentration of a solute in aqueous solution.

Syllabus subject matter

Topic 2 • Aqueous solutions and acidity

■ AQUEOUS SOLUTIONS AND MOLARITY

- Explain that the unique properties of water are related to molecular shape and hydrogen bonding between molecules. **13.1**
- Discriminate between the terms *solute*, *solvent*, *solution*. **13.2**
- Discriminate between unsaturated, saturated and supersaturated solutions. **13.3**
- Apply the mole concept to calculate moles of solute, concentration and volume of a solution.

$$\left(\text{Formula: molarity / concentration } (c) = \frac{\text{moles of solute } (n)}{\text{volume of solution } (V)}\right) \textbf{ 13.5}$$

■ IDENTIFYING IONS IN SOLUTION

- Apply ionic and chemical formulas to construct balanced ionic and chemical equations (including states) for precipitation reactions. **13.4**
- Apply solubility rules to predict if a precipitation will be formed. **13.4**
- Analyse data, including precipitation and acid-carbonate reactions, to determine the presence of specific ions in solutions.* **13.4**

SOLUBILITY

- Compare the solubility of ionic and molecular substance in water, and the intermolecular forces between species in the substances and water molecules. **13.2**
- Identify that changes in solvent temperature can affect the solubility of solid and gaseous solutes (solids and gases). **13.3**
- Analyse data, including solubility curves, to determine the solubility of ionic compounds and the concentration of ions in aqueous solutions. **13.3**

*The greyed-out section of this dot point is addressed explicitly in another chapter.

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13.1 Structure and properties of water

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- identify the unique properties of water, including its boiling point, surface tension and density
- explain that the unique properties of water are related to molecular shape and hydrogen bonding between molecules.

Water is a special chemical. It moderates our weather, shapes our lands and is essential for the existence of life. Water is the most abundant liquid on Earth, covering more than 70% of our planet. The total water supply is estimated to be more than 1.3 billion cubic kilometres.

This water on Earth constantly cycles, as shown in Figure 13.1.1. It is in continuous movement between land, ocean, rivers and creeks and the atmosphere. Warmth from the sun causes the water in oceans, lakes and rivers to evaporate and become vapour in the air. As water vapour rises, the air temperature drops and the water vapour condenses to form droplets, which merge to form clouds. When the water droplets are large enough, water falls back to Earth as rain, ice or snow, depending on the air temperature. Other processes also add water to the atmosphere. When fossil fuels undergo combustion, water is a product and is released into the air. Water also evaporates from the leaves, stems and flowers of plants.

FIGURE 13.1.1 The water cycle. The arrows show some of the ways water on Earth is redistributed.

Water and life are so strongly linked that space scientists search the universe for water in their quest to discover possible life beyond our planet. It is the unique properties of water that allow it to support life.

These properties can be explained by looking at the structure of a water molecule and the **hydrogen bonding** that occurs between the water molecules.

WATER AND HYDROGEN BONDING

Structure of water

Water has the chemical formula H_2O, which means that each water molecule contains two hydrogen atoms and one oxygen atom. As you will recall from Chapter 8, hydrogen and oxygen are both non-metals so they bond with each other by sharing electrons. Each hydrogen atom shares one electron with the oxygen atom and the oxygen atom shares one electron with each hydrogen atom. The sharing of electrons means these **intramolecular bonds** are covalent.

Each oxygen atom also has two **lone pairs** (non-bonding pairs) of electrons that contribute to the molecule's shape. A water molecule is bent as shown in Figure 13.1.2. The lone pairs of electrons on the oxygen atom have greater repulsion than the electrons forming the single bonds between oxygen and hydrogen. This pushes the hydrogen atoms closer together, giving the overall bent shape (the shape of molecules was explained in detail in Chapter 11).

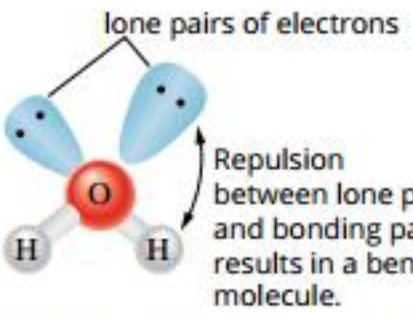


FIGURE 13.1.2 In this diagram of the valence structure of water, the two hydrogen atoms (white) form a bent shape with a central oxygen atom (red).

The covalent bonds in a water molecule are **polar**. The oxygen atom has a higher **electronegativity** than the hydrogen atoms. This means that the electrons in the O–H bonds are more strongly attracted to the oxygen atom. Uneven sharing of the electrons gives the oxygen atom a partial negative charge (δ-) and each hydrogen atom carries a partial positive charge (δ+).

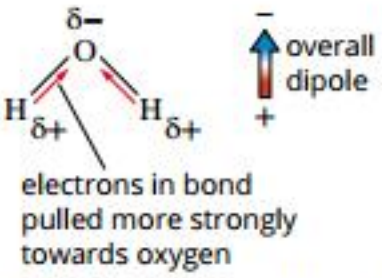


FIGURE 13.1.3 A water molecule has an overall dipole. The oxygen atom has a partial negative charge, while the hydrogen atoms both have partial positive charges.

Since the bonding electrons are distributed unevenly across the water molecule, the molecule can be described as polar. Figure 13.1.3 shows how the individual **dipoles** of the O–H bonds in water add together, resulting in an overall molecular dipole.

Polar bonds and polar molecules were explained in detail in Module 11.2.

Hydrogen bonding between water molecules

The main type of **intermolecular force** between molecules of water is the **hydrogen bond**. The hydrogen bonds are formed by an **electrostatic attraction** between the partial positive charge on a hydrogen atom on one water molecule and a lone pair of electrons on the oxygen atom of a neighbouring water molecule.

Figure 13.1.4 shows the hydrogen bonding between molecules of water. Each water molecule is colour-coded to show its polarity. The two hydrogen atoms in each water molecule have a slight positive charge (white), while the central oxygen atom has a slight negative charge (red). The black dashed lines represent the hydrogen bonds that form between water molecules. (For more details on hydrogen bonding, see Module 11.3.)

Water molecules are polar and have a permanent overall dipole.

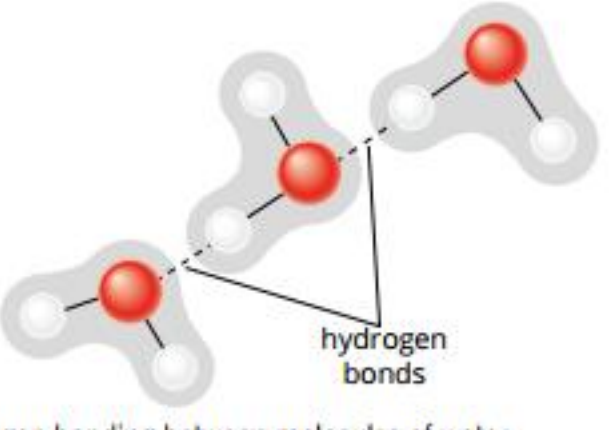


FIGURE 13.1.4 The hydrogen bonding between molecules of water

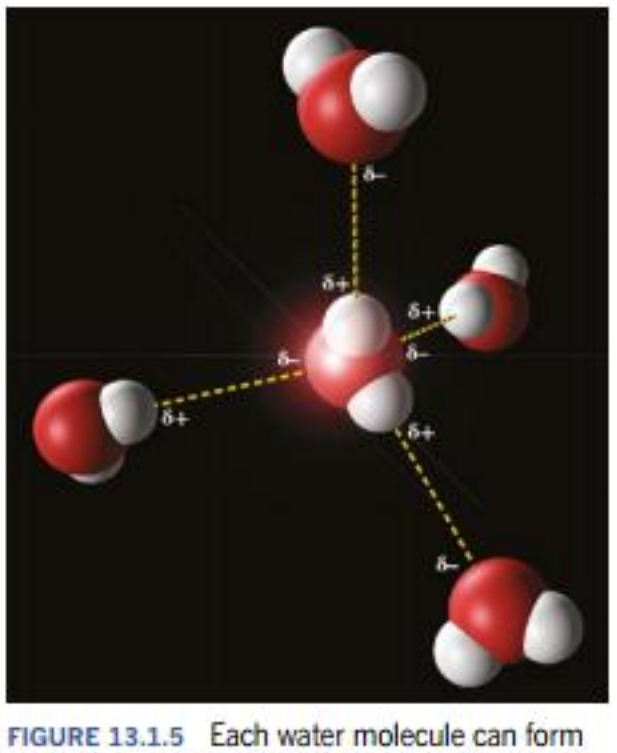


FIGURE 13.1.5 Each water molecule can form hydrogen bonds to four other water molecules.

Because there is a large electronegativity difference between oxygen and hydrogen atoms, the partial charges on a water molecule are relatively large. The electrostatic attraction between these opposite partial charges on neighbouring molecules makes the hydrogen bonds between water molecules quite strong.

As Figure 13.1.5 shows, each water molecule can form hydrogen bonds with up to four other water molecules.

MELTING AND BOILING POINTS OF WATER

Compared to other molecules of a similar size, water has high boiling and melting points. This can most easily be seen through the observed trends in these properties for the group 16 hydrides.

Trends in group 16 hydrides

The group 16 elements include oxygen (O), sulfur (S), selenium (Se), tellurium (Te) and polonium (Po). Each of these elements can bond with hydrogen to form compounds known as **hydrides**. Water is a group 16 hydride. The group 16 hydrides are listed in Table 13.1.1.

TABLE 13.1.1 Names and formulas of the group 16 hydrides

Element	Name and formula of hydride	Formula
O	water	H_2O
S	hydrogen sulfide	H_2S
Se	hydrogen selenide	H_2Se
Te	hydrogen telluride	H_2Te
Po	hydrogen polonide	H_2Po

The group 16 hydrides are all molecular compounds, so their melting and boiling points reflect the size of the forces between their molecules. The higher the melting and boiling points, the stronger the intermolecular forces must be because more energy is required to overcome the forces and allow the molecules to move apart from each other.

The melting and boiling points of the group 16 hydrides are shown in Table 13.1.2 and Figure 13.1.6.

TABLE 13.1.2 Melting and boiling points of the group 16 hydrides

Hydride	Molar mass ($g\,mol^{-1}$)	Melting point (°C)	Boiling point (°C)
H_2O	18.0	0	100
H_2S	34.1	−82	−60.7
H_2Se	81.0	−66	−41.5
H_2Te	129.6	−49	−2.2
H_2Po	212.0	−35	36.1

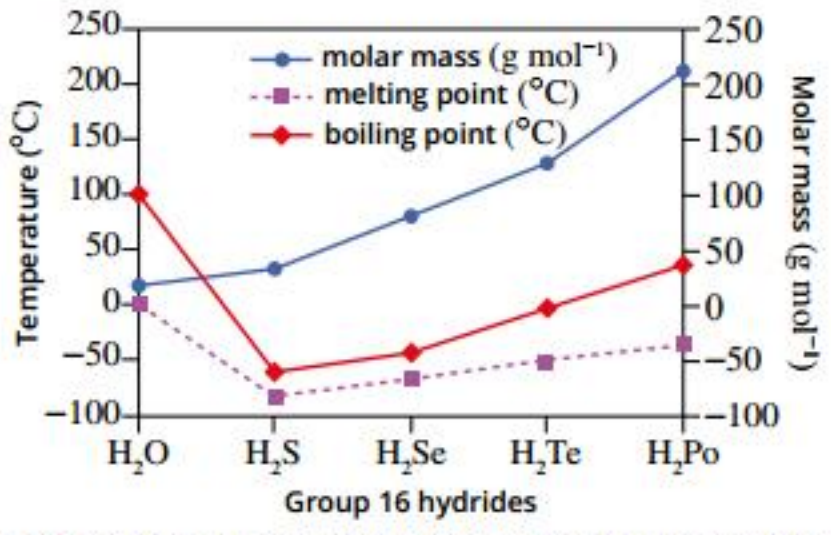


FIGURE 13.1.6 Graph showing the trend in molar mass, melting point and boiling point of water and other group 16 hydrides

Each water molecule has the potential to form four hydrogen bonds with surrounding water molecules. There are two partially charged hydrogen atoms and two lone pairs of electrons on the oxygen atom in each molecule, so all the hydrogen atoms and lone pairs in the molecule can be involved in hydrogen bonding with areas of opposite charge on another molecule.

You can see from Figure 13.1.6 that, apart from water, there are clear trends in the melting and boiling points of the group 16 hydrides. With the exception of water, melting and boiling points increase going down the group. This increase indicates that the intermolecular forces are also getting stronger down the group. As you learnt in Chapter 11, the intermolecular forces responsible for this trend are dispersion forces. Dispersion forces increase in strength with increasing molar mass. H_2Po has a larger molar mass than H_2S and H_2Se; hence it has stronger dispersion forces and higher melting and boiling points.

The melting and boiling points of water are exceptional

Water has a melting point of 0°C and a boiling point of 100°C. Both of these values are significantly higher than those of other group 16 hydrides. The values are also significantly higher than those of other molecular substances of a similar molar mass, as can be seen in Figure 13.1.7.

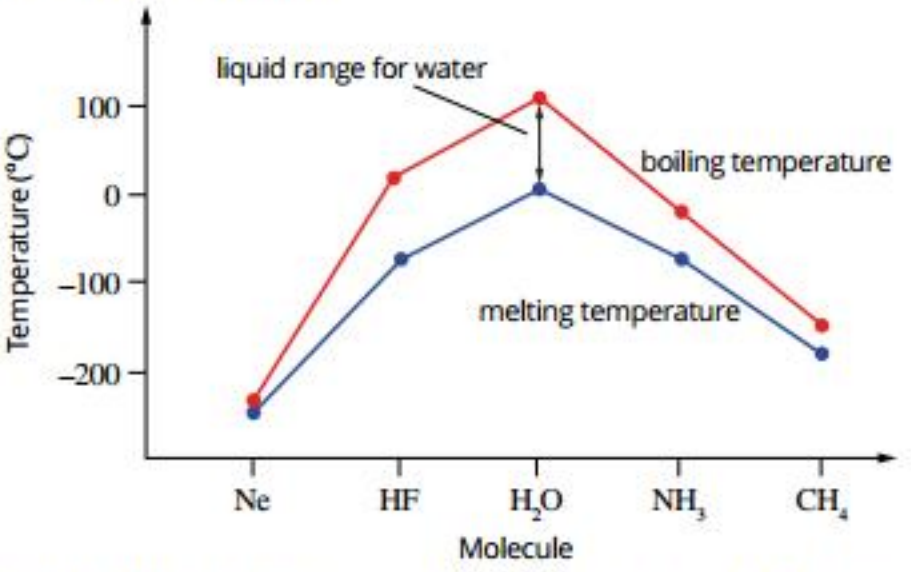


FIGURE 13.1.7 The melting and boiling points of water and other molecules of similar size

It is the relatively strong hydrogen bonds between its molecules that give water its exceptional properties.

A significant amount of energy is needed to disrupt all of the hydrogen bonds between water molecules, resulting in the higher melting points and boiling points observed for water.

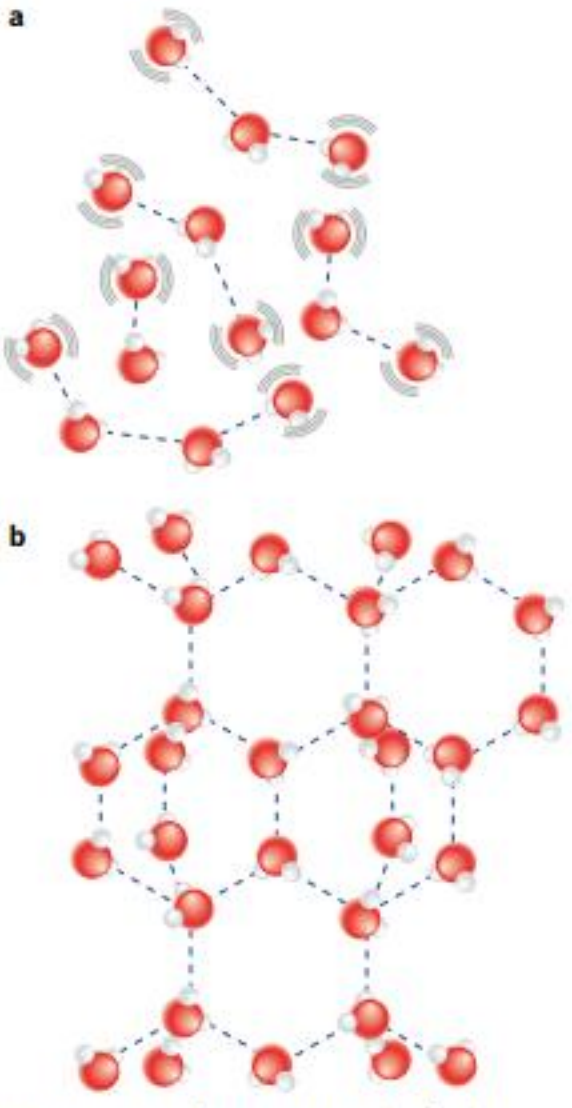


FIGURE 13.1.8 The arrangement of water molecules (a) in liquid water and (b) ice

DENSITY IN LIQUID AND SOLID STATES

Density is a characteristic property of a substance and is the measure of the mass of a substance within its volume. It is usually measured in grams per cubic centimetre. The nature of the bonding and intermolecular forces between molecules will affect the density of a substance, and water in the liquid and solid states is quite unique.

Water expands on freezing

When a sample of water freezes, the resulting ice crystal lattice has a greater volume than when the sample of water was a liquid. Water has the unusual property of having a lower density in the solid phase than in the liquid phase.

This property of water is important to life on Earth. When water at the surface of rivers or lakes freezes, the low density of the ice means it remains on the surface. This surface layer of ice insulates the water below from the cold air temperatures, reducing the possibility that the entire river or lake will freeze, and allowing aquatic life to survive.

As liquid water is cooled, the water molecules move more slowly. Upon approaching the freezing temperature of water, the molecules become arranged in a way where each water molecule forms four hydrogen bonds to four neighbouring water molecules, as shown in Figure 13.1.8.

This creates a very open arrangement of molecules, meaning that the water molecules in ice are more widely spaced than in liquid water. Therefore, ice is less dense than liquid water. When ice melts, the water molecules move more freely and move closer together.

SPECIFIC HEAT CAPACITY

Several of the ways in which water supports life on Earth are based on how water interacts with heat energy. When you walk on the beach on a hot summer's day, the dry sand can be burning hot on your feet while the shallow water at the edge of the sea is cool. Both surfaces are receiving and absorbing similar amounts of heat energy from the sun, but the temperature of each is markedly different. Water has a higher specific heat capacity than sand, meaning water can absorb a relatively large quantity of heat energy for very small changes in temperature.

Recall from Module 10.3 that the **specific heat capacity** of a substance measures the amount of energy (in joules) needed to increase the temperature of 1 gram of that substance by 1°C.

Specific heat capacity is given the symbol c and is expressed in joules per gram per degree Celsius, $J g^{-1} °C^{-1}$.

The specific heat capacities of some common substances are shown in Table 13.1.3. You can see that the value for water is high. It takes more energy to increase the temperature of water compared to other substances.

TABLE 13.1.3 Heat capacities of some selected substances

Substance	Specific heat capacity ($J g^{-1} °C^{-1}$)
aluminium	0.90
copper	0.39
concrete	0.80
ethanediol (antifreeze)	2.42
glass	0.84
iron	0.45
water	4.18

The specific heat capacity of a substance is a reflection of the type of bonds holding molecules, ions or atoms together in the substance. The relatively high specific heat capacity of water is related to the number and strength of the hydrogen bonds between water molecules. Hydrogen bonds are stronger than other intermolecular forces and they are able to absorb and store large amounts of heat energy before they are disrupted.

The specific heat capacity of a substance reflects the type of bonding in that substance. For molecular substances such as water, the heat capacity will depend on the strength of the forces between molecules (intermolecular forces).

LATENT HEAT

When you perspire (sweat), your body uses a very effective method to cool down. The water released onto your skin as sweat sits on the surface of the skin and absorbs relatively large amounts of heat energy from the body before it evaporates as a gas. In combination with its high specific heat capacity, it is the **latent heat** of water that makes it such an effective coolant.

When a solid is heated at constant pressure, the temperature of the solid increases until it reaches its melting point. The temperature then remains constant as the solid melts, even though further energy is being absorbed. Similarly, when a liquid reaches its boiling point, its temperature remains constant as boiling occurs until all of the liquid has evaporated. Figure 13.1.9 on page 346 shows the temperature of water as it is heated over time. No matter how long the water is heated, the temperature of the liquid water never rises above 100°C; its temperature only rises higher after it has all become gaseous. This is because the heat energy being supplied is being used to change the state of the water (from liquid to gas).

Even though the temperature does not change while a phase change is taking place, the substance is still absorbing energy. This energy is referred to as latent heat and is defined as the energy absorbed by a fixed amount of substance as it changes state from a solid to a liquid or a liquid to a gas at its melting point or boiling point respectively.

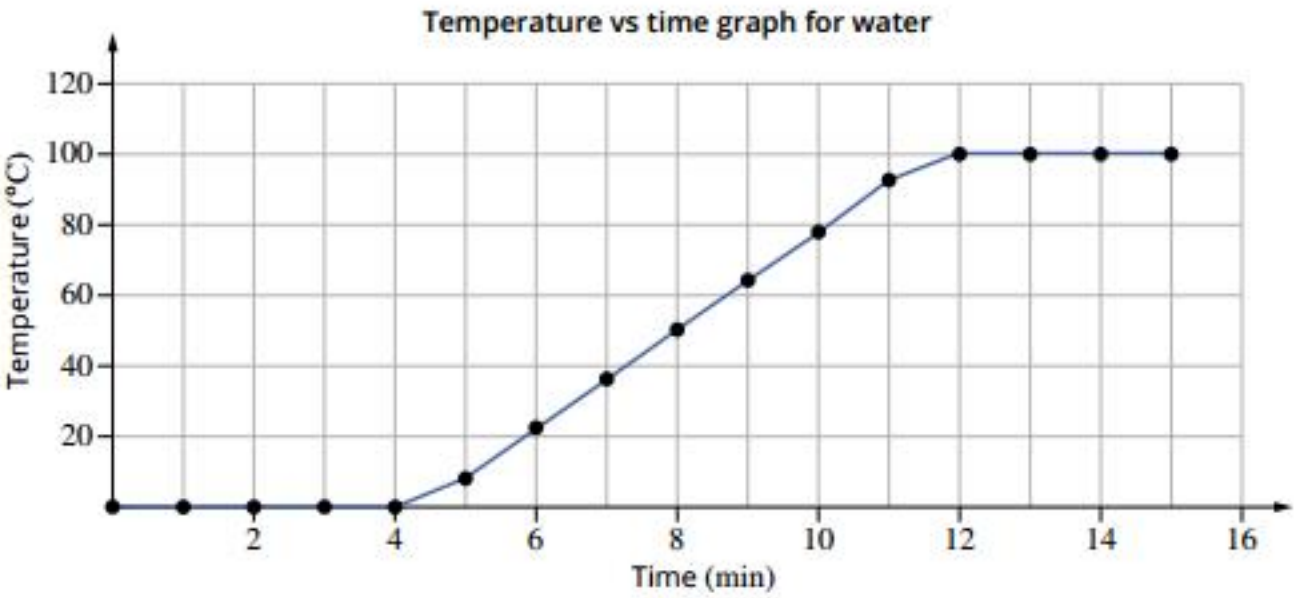


FIGURE 13.1.9 A temperature versus time graph for water, showing the plateaus at 0°C and 100°C

Latent heat is the energy required to change a fixed amount of substance, usually 1 mole, from either a solid to a liquid at melting point or from a liquid to a gas at boiling point. Over the period of time that latent heat is being absorbed, the temperature of a substance will not change.

Values of latent heat

Latent heat values are a measure of the quantity of heat energy required to melt or boil a given amount of a solid or liquid. Latent heat values have the unit kilojoules per mole, $kJ\,mol^{-1}$.

The **latent heat of fusion** of a substance is the energy needed to change 1 mole of the substance from a solid to a liquid at its melting point.

The **latent heat of vaporisation** of a substance is the energy needed to change 1 mole of the substance from a liquid to a gas at its boiling point.

Latent heat of water

The latent heat of fusion of water is $6.0\,kJ\,mol^{-1}$. This means that 6.0 kJ of energy is needed to change 1 mole of water from a solid to a liquid at 0°C. This energy is needed to disrupt the ice lattice by breaking some of the hydrogen bonds between water molecules.

The latent heat of vaporisation of water is $40.7\,kJ\,mol^{-1}$. This means that 40.7 kJ is needed to change the state of 1 mole of water from a liquid to a gas at 100°C. This relatively large quantity of energy is required to completely break the hydrogen bonds between the water molecules so they can separate and form a gas.

The latent heat values of water and some other substances are listed in Table 13.1.4. Like specific heat capacity, latent heat depends on the strength of the forces between molecules of the substance (intermolecular forces).

TABLE 13.1.4 Latent heat values for some common molecular substances

Substance	Latent heat of fusion ($kJ\,mol^{-1}$)	Latent heat of vaporisation ($kJ\,mol^{-1}$)
water	6.0	40.7
hydrogen	0.06	0.45
oxygen	0.22	3.4

As you can see, the latent heat values of water are relatively high. This is due to the strength and number of water's hydrogen bonds relative to its molecular size.

Regulation of ocean temperatures

Ocean temperatures vary throughout ocean waters across Earth. The average temperature of Earth's water at the ocean surface is about 17°C. The Indian Ocean has the warmest temperatures, ranging from 19°C to 30°C, while the Arctic Ocean is the coldest at around 2.2°C. Although there is variation in ocean temperatures around the globe, the temperature of each individual region stays relatively stable.

This is important for aquatic marine life as large fluctuations in temperature can cause them harm. It is water's high latent heat value of vaporisation and its high specific heat capacity that aid temperature regulation. Water's high specific heat capacity means high levels of sunlight do not result in large increases in water temperature, and its high latent heat value means that high levels of sunlight do not result in excessive evaporation.

SURFACE TENSION

The water molecules at the surface of a sample of water are not completely surrounded by other water molecules. As a result, they form hydrogen bonds with neighbouring molecules on the sides and below, but not above.

The sideways forces of attraction to neighbouring molecules are equal in all directions, so for molecules in the body of the liquid, there is no net force. However, the attraction of surface water molecules to the molecules below them has no opposite force, so the water molecules at the surface are pulled downwards.

In a beaker of water at room temperature, a water molecule will spend, on average, only 10^{-9} seconds or 1 nanosecond at the surface before being pulled back into the bulk of the liquid (Figure 13.1.10). The surface of the water is in a constant state of tension.

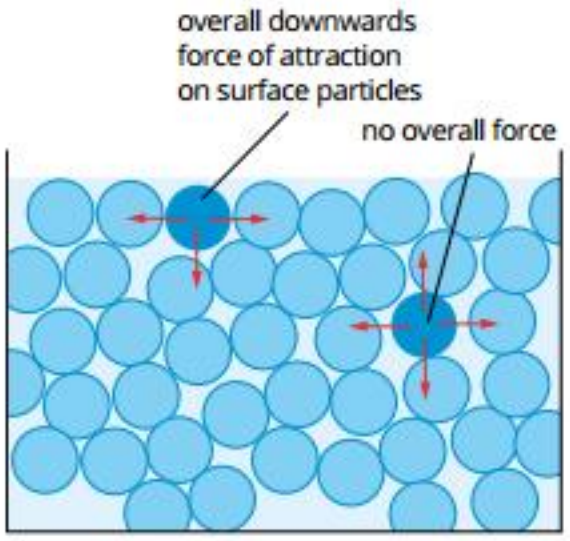


FIGURE 13.1.10 Forces of attraction on particles at the surface and in the body of a liquid. The particles in the body of the liquid experience no net force. The particles at the surface of the liquid have an overall downwards force of attraction.

Water, with relatively strong hydrogen bonds between molecules, has a relatively high **surface tension**. The surface tension of a substance is a measure of the resistance of a liquid to increasing its surface area. The surface tension is why falling water tends to form droplets. It also explains why insects are able to walk across water.

You can see in Figure 13.1.11 that the surface of the water behaves like a stretched skin. The water molecules at the surface are so attracted to each other by strong hydrogen bonds that the paperclip floats, even though the density of the paperclip is higher than the density of water.

FIGURE 13.1.11 The relatively high surface tension of water allows this paperclip to float.

13.1 Review

SUMMARY

- A water molecule has a bent shape and contains polar covalent bonds.
- Water molecules are polar because an overall dipole exists as a result of the unsymmetrical nature of the polar O–H bonds.
- The forces that attract one water molecule to another are relatively strong hydrogen bonds.
- Each water molecule can form up to four hydrogen bonds with other water molecules.
- The strength of water's hydrogen bonds means relatively large amounts of energy are required to disrupt the bonds and separate the molecules from each other. This gives water relatively high melting and boiling points.
- Water has significantly higher melting and boiling points than the other group 16 hydrides.
- With the exception of water, the melting and boiling points of the group 16 hydrides increase going down the group. This is due to the increasing strength of dispersion forces.
- Ice is less dense than liquid water because of its unique geometric arrangement of water molecules as a result of hydrogen bonding.
- Heat capacity is a measure of a substance's capacity to absorb and store heat energy.
- When compared to other substances, water has a high specific heat capacity of $4.18\,J\,g^{-1}\,°C^{-1}$.
- The high specific heat capacity of water is due to the ability of the hydrogen bonds between water molecules to absorb and store heat energy.
- Latent heat is the energy absorbed by a fixed amount of substance as it changes state from a solid to a liquid or a liquid to a gas.
- The latent heat of fusion of a substance is the heat energy needed to change 1 mole of a substance from a solid to a liquid at its melting point.
- The latent heat of vaporisation of a substance is the heat energy needed to change 1 mole of a substance from a liquid to a gas at its boiling point.
- Water's high values for latent heat of vaporisation and specific heat capacity help to regulate ocean temperatures and preserve water supplies.
- The attraction of surface water molecules to the molecules below them has no opposite force, so the water molecules at the surface are pulled downwards, creating a high surface tension.

KEY QUESTIONS

Describe

1 List the physical properties that make water unique.

2 Ice is less dense than water. Describe the bonding formed between water molecules in ice that means solid water is less dense.

3 What is the definition of specific heat capacity?

4 Why are the water molecules at the surface of water pulled downwards, generating surface tension, yet molecules in the body of the liquid do not show this?

5 Explain why water can form hydrogen bonds and dipole–dipole interactions with other molecules.

6 What type of bonding is responsible for water's relatively high latent heat values?

Apply

7 Table 13.1.3 on page 345 shows the specific heat capacities of some substances. Order the substances from the one that absorbs the least amount of energy to the one that absorbs the most for the same increase in temperature.

8 Explain why water's latent heat of vaporisation is much higher than its latent heat of fusion.

9 Explain the significance of polarity and hydrogen bonding in relation to the high melting and boiling points of water, and its density.

Analyse

10 Explain why a water molecule can form up to four hydrogen bonds with other water molecules.

11 With the exception of water, the group 16 hydrides exhibit a trend in boiling and melting points.

a Sort the group 16 hydrides (H_2O, H_2Po, H_2S, H_2Se, H_2Te) from lowest to highest boiling point.

b Explain why water does not follow the trend of the other group 16 hydrides.

12 Detergents are known to lower the surface tension of water. Determine the implications to aquatic organisms of detergents leaching into natural waterways.

13.2 Water as a solvent

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- discriminate between the terms solute, solvent, solution
- compare the solubility of ionic and molecular substances in water, and the intermolecular forces between species in the substances and water molecules.

Water is an excellent solvent. This is one of its most important properties. Almost all biological processes and many industrial processes occur in water. These systems are known as **aqueous** environments.

When substances are dissolved in water, the particles are free to move throughout the **solution**. When two aqueous reactants are combined in a reaction vessel, the dissolved reactant particles mix freely. This increases the chances of the reactants coming into contact. Because of the increased movement of the reactant particles, interactions between reactants are generally much more effective than if the same reactants were mixed as solids.

In Figure 13.2.1, you can see how the deep purple colour of potassium permanganate spreads through the water as the solid dissolves. Eventually the liquid will appear completely purple as the particles continue to mix and move.

This module explores the process of dissolving in more detail, including a description of the types of bonds that form when molecular and ionic substances dissolve in water.

FIGURE 13.2.1 When solid potassium permanganate is added to water, it dissolves. The particles disperse into the solution and move around freely.

FORCES BETWEEN SOLUTE AND SOLVENT PARTICLES

An aqueous solution is formed when a solid, liquid or gas is dissolved in water. The substance being dissolved is called the **solute** and the liquid in which the substance is dissolved is the **solvent**. When a solute dissolves, the forces holding the solute together, and the **forces** holding the water molecules together, must be broken. New forces of attraction between the solute and solvent can then form.

Aqueous solutions

The solute of an aqueous solution can change but the solvent will always be water. You can have an aqueous solution of salt (saline) or an aqueous solution of sugar. Table 13.2.1 lists some common aqueous solutions.

TABLE 13.2.1 Some everyday aqueous solutions

Solution	Solute/s	Solvent
saline solution (for use with contact lenses)	sodium chloride	water
soft drink	carbon dioxide, sugar, flavour, colour	water
coffee	coffee, sugar	water

All solutions have the following characteristics.

- The solute and the solvent cannot be distinguished from each other. This means the solution is **homogeneous**.
- The dissolved particles are too small to see.
- The amount of dissolved solute can vary from one solution to another.

In a homogeneous solution, the solute and solvent particles cannot be distinguished from each other. Every part of the solution is the same as any other part.

Process of dissolving

The process of a substance dissolving in another substance is called **dissolution**. When the two substances are liquids, you can say they are **miscible**.

During dissolution the following processes occur.

- The particles of the solute are separated from one another.
- The particles of the solvent are separated from one another.
- The solute and solvent particles are attracted to each other.

For a solution to form, the solute particles must interact with the solvent molecules. The solute particles are surrounded by solvent molecules and carried throughout the solution.

Forces in dissolving

For a substance to dissolve, there must be a change in the way particles in the solute and solvent interact. This means you need to look at the forces of attraction that occur between the particles.

It is useful to think of three different forces of attraction when considering if and how a substance will dissolve in water. These are the forces that:

- hold the particles of the substance (solute) together before it is added to the solvent; for example, ionic bonds or intermolecular forces
- hold the solvent molecules together; in water, these forces are **hydrogen bonds and dispersion forces**
- form between the solute particles and solvent molecules if the substance dissolves.

For a substance to dissolve, the attractive forces that form between the solute and solvent particles must be similar to or greater than the forces between the particles in the solute and the forces between the solvent molecules.

Figure 13.2.2 shows that as a solute dissolves, the solute particles separate and become evenly distributed in the solvent. If the attraction between the solute and solvent particles is not strong enough, then the substance will not readily dissolve.

i For a substance to be soluble, the solute–solvent interactions must be stronger than the solute–solute and solvent–solvent interactions.

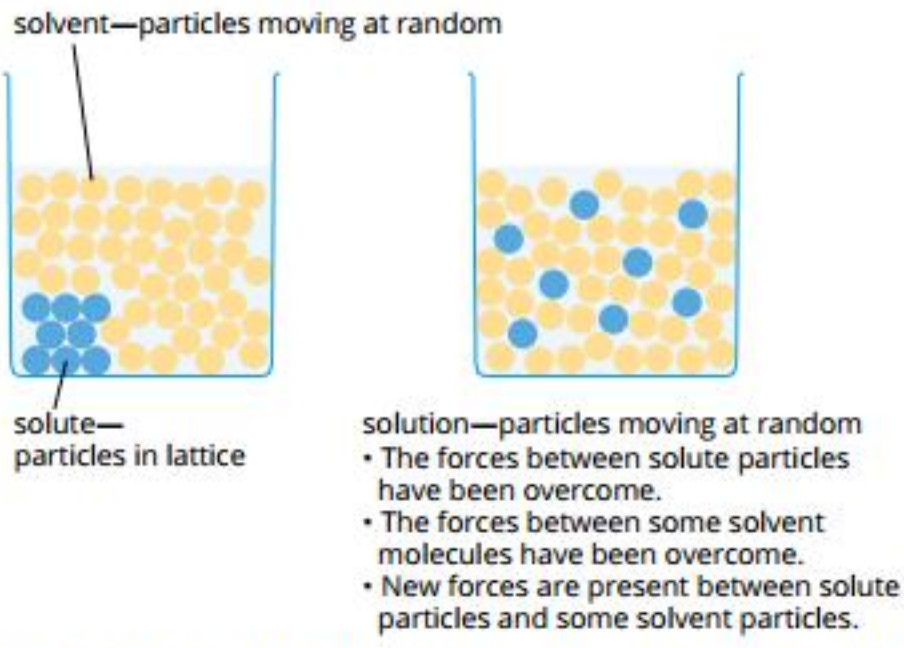

solvent—particles moving at random
solute—
particles in lattice
solution—particles moving at random
• The forces between solute particles have been overcome.
• The forces between some solvent molecules have been overcome.
• New forces are present between solute particles and some solvent particles.

FIGURE 13.2.2 The rearrangement of particles when a solute dissolves in a solvent. The solute particles separate and become evenly distributed in the solvent.

Like dissolves like

You can use a 'like dissolves like' rule to predict whether a substance is likely to dissolve in another substance. The general statement that a solvent will only dissolve 'like' solutes tells you that:

- polar solvents will generally dissolve substances consisting of polar molecules or charged ions, but will not dissolve solutes made up of **non-polar** molecules
- non-polar solvents can dissolve substances consisting of non-polar molecules, but will not dissolve ones with polar molecules or ions.

Oil and other non-polar molecular substances do not dissolve well in water because the only intermolecular forces in these substances are dispersion forces, whereas the strong intermolecular forces of hydrogen bonding exist between the water molecules. These hydrogen bonds between water molecules are much stronger than the dispersion forces that could occur between molecules of oil and water. As a result, the attraction between the water molecules cannot be overcome and the water molecules do not separate to form a solution with the oil molecules.

You can observe the 'like dissolves like' rule with the miscibility of different liquids. Figure 13.2.3 shows a solution of ethanol and water. The polar nature of the ethanol molecule means it readily dissolves in water, which is also polar. When mixed, a homogeneous solution is formed with no separation between solute and solvent.

In contrast, hexane is **immiscible** in water. Hexane is composed of non-polar molecules that will not interact with the polar water molecules. Figure 13.2.4 shows that when hexane and water are mixed, two layers form and the less dense hexane sits on top of the water.

Like hexane, olive oil is also composed of non-polar molecules. When olive oil and hexane are mixed with each other, the 'like dissolves like' rule applies and the two non-polar liquids readily mix with each other to form a homogeneous solution (Figure 13.2.5).

Use the 'like dissolves like' principle to predict if a substance will dissolve in a solvent.

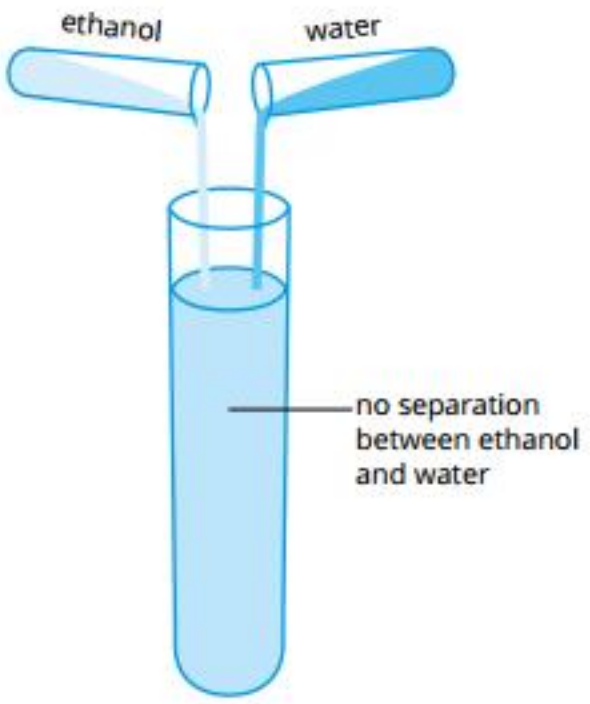


FIGURE 13.2.3 The polar compound ethanol is completely miscible in water. A homogeneous solution is formed on mixing.

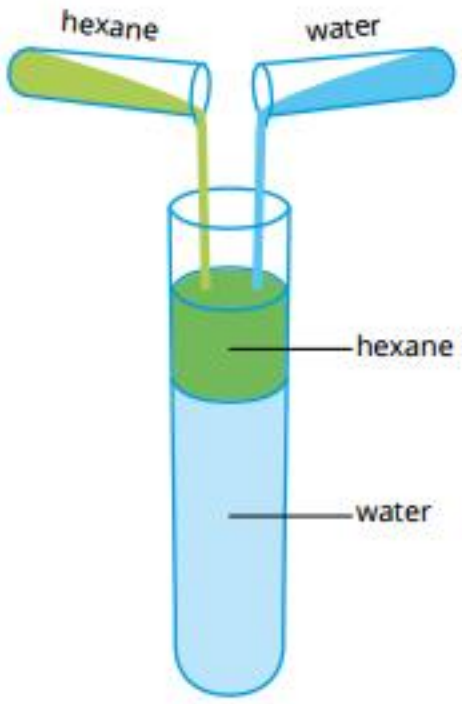


FIGURE 13.2.4 Hexane is a non-polar molecular compound that is not miscible in water. Two layers are formed with the non-polar liquid sitting on top of the water layer.

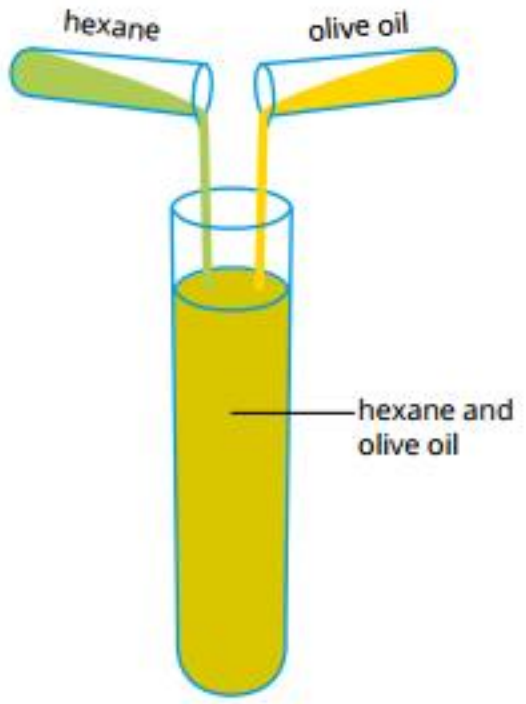


FIGURE 13.2.5 Hexane and olive oil are both non-polar molecular compounds and so are completely miscible.

DIFFERENT WAYS COMPOUNDS DISSOLVE IN WATER

The way a compound dissolves depends on the bonding present in the substance. Most molecular substances are insoluble (or only very slightly soluble) in water. However, some smaller molecules, such as ammonia (NH_3), hydrogen chloride (HCl) and sugar ($C_{12}H_{22}O_{11}$) dissolve well in water. Solutions in which a molecular substance is at least one of the solutes include brick cleaner, various liquid fertilisers and drinks such as wine and cordial.

Many, but not all, ionic substances are soluble in water. Seawater contains dissolved sodium chloride and other dissolved ions, such as magnesium, calcium, bromide and sulfate ions.

There are three main ways that compounds dissolve in water:

- Some molecular compounds dissolve by forming hydrogen bonds with water.
- Other molecular compounds dissolve in a process that involves the formation of ions.
- Ionic compounds dissolve in a process where the ions break away from the lattice.

Molecular compounds that can form hydrogen bonds are often soluble in water.

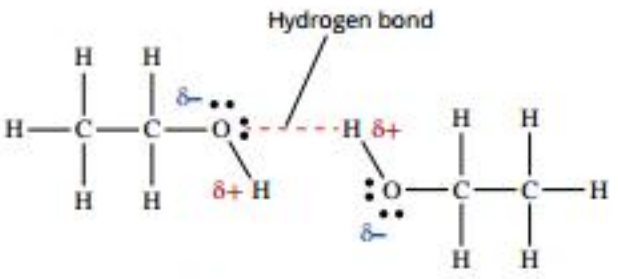


FIGURE 13.2.6 Hydrogen bonding in pure ethanol. The intermolecular hydrogen bond is formed between the lone pair electrons on the oxygen atom of one ethanol molecule and the electron-deficient hydrogen atom of an adjacent ethanol molecule.

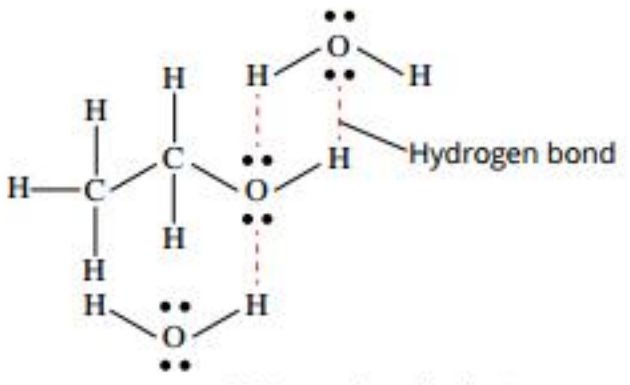


FIGURE 13.2.7 Hydrogen bonding between ethanol and water

When a polar molecular substance dissolves in water by forming hydrogen bonds, the equation for dissolution places water above the arrow.

Molecular compounds that form hydrogen bonds with water

One way a molecular compound might dissolve in water is if its molecules form hydrogen bonds with water molecules. An example of such a molecule is ethanol.

Ethanol (C_2H_5OH) is a liquid at room temperature. Its molecules contain the polar -OH group, with lone pairs of electrons on the oxygen atom. The presence of the hydrogen atoms bonded to the more electronegative oxygen atom allows an ethanol molecule to form hydrogen bonds.

Figure 13.2.6 shows how hydrogen bonds form between molecules in pure ethanol.

When ethanol is added to water, it dissolves. The two liquids are miscible. Figure 13.2.7 shows how hydrogen bonds form between the ethanol and surrounding water molecules.

Because the strength of the solute–solute intermolecular forces is similar to the strength of the solute–solvent intermolecular forces, the two substances can readily interact with each other. Therefore, water and ethanol molecules mix freely with each other, held together in solution by hydrogen bonds.

In summary, when ethanol dissolves in water, hydrogen bonds between:

- water molecules break
- ethanol molecules break
- ethanol molecules and water molecules form.

An equation for the dissolution of ethanol can be written to represent this process:

$$C_2H_5OH(l) \xrightarrow{H_2O(l)} C_2H_5OH(aq)$$

Note that the formula of water sits above the arrow. This is because there is no direct reaction between the water and the ethanol. The two substances simply mix together. No chemical change occurs; only the state symbol for ethanol is altered from (l) to (aq), indicating it is now dissolved in water.

Like ethanol, sugars such as glucose, fructose and sucrose also contain the polar –OH group and can therefore dissolve in water by forming hydrogen bonds. The structure of each of these sugars is shown in Figure 13.2.8. Each of the –OH groups in the molecule can form hydrogen bonds with water molecules. Because each molecule has many –OH groups, sugars are very soluble in water.

The more polar the molecules of a molecular compound are, the more likely the compound is to dissolve in water. Some molecules have a polar section and a non-polar section. In general, the larger the non-polar section of the molecule, the less soluble it is in water.

Carboxylic acids are a type of organic molecule that have a hydrocarbon chain of varying length and a carboxyl functional group. The carboxyl functional group contains a carbon double-bonded to an oxygen and a bond to a hydroxyl functional group. It is often written as –COOH. The presence of the hydroxyl (–OH) functional group makes this end of the molecule polar. However, the hydrocarbon chain is non-polar due to the symmetrical nature of the hydrocarbon chain. Therefore, the longer the chain, the more non-polar the molecule is. Therefore, the **solubility** of carboxylic acids and alcohols is largely dependent on the size of the hydrocarbon chain to which it is attached.

Non-polar molecular substances do not have charged ends so there is no significant attraction to water molecules. The only forces of attraction that exist between non-polar substances and water are weak dispersion forces, which are not strong enough to overcome the relatively strong hydrogen bonding between water molecules.

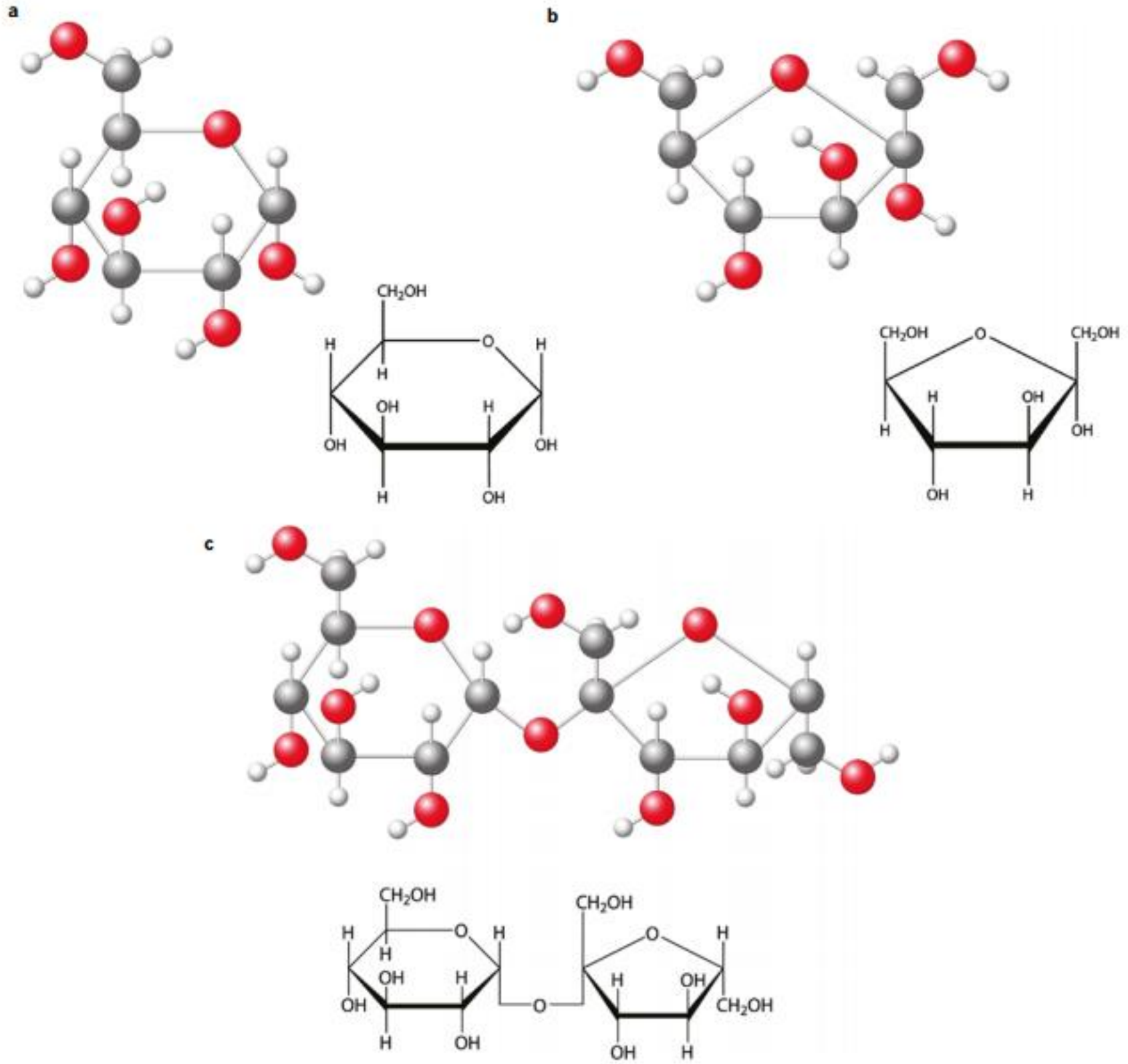
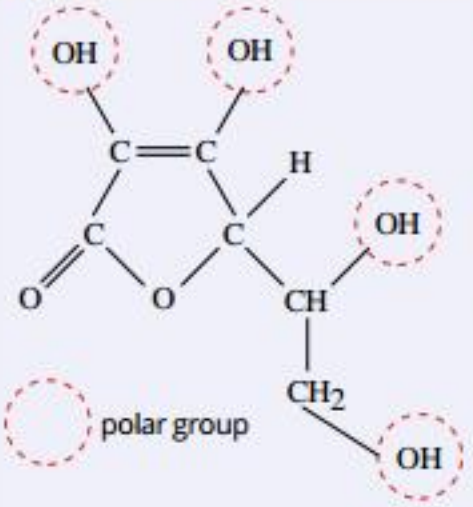
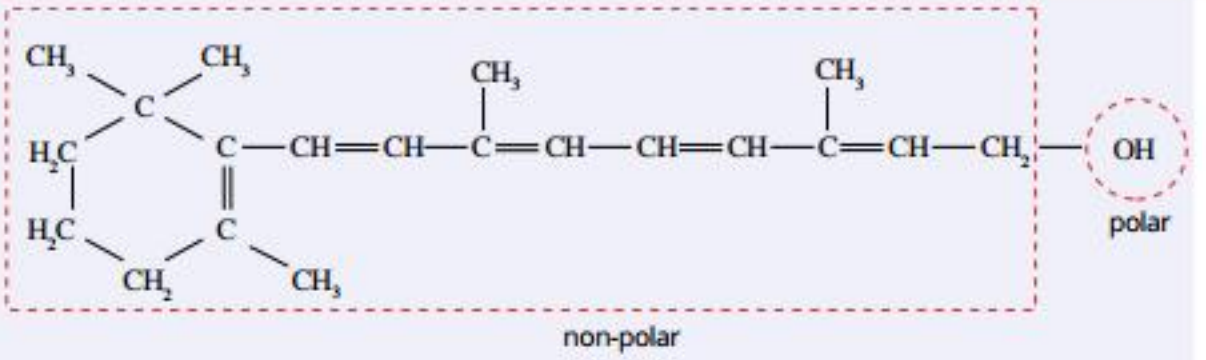


FIGURE 13.2.8 These are the molecular structures of common sugars: (a) glucose (the sugar found in our blood), (b) fructose (fruit sugar) and (c) sucrose (table sugar—the sugar used to sweeten tea and coffee). Each of these sugars can dissolve in water because of the presence of polar –OH groups.

Table 13.2.2 on page 354 compares the structures and properties of vitamin C and vitamin A. Both molecules contain the polar –OH group, but only vitamin C is soluble in water. The higher proportion of polar –OH groups on the vitamin C molecule allows it to form sufficient hydrogen bonds with water to overcome the strong attraction between water molecules, therefore dissolving to form a solution.

TABLE 13.2.2 Comparison of the solubility and structures of vitamin C and vitamin A

	Vitamin C	Vitamin A
structure	 Vitamin C: • contains four polar O–H groups • molecule quite polar.	 Vitamin A: • contains one polar O–H group • molecule largely non-polar.
solubility	highly soluble in water, insoluble in fats	soluble in fats, insoluble in water
biological significance	The high solubility of vitamin C means it is excreted in urine so it must form a regular part of the diet.	Vitamin A is not excreted in urine but is stored in body fat. The body can tolerate a diet low in vitamin A for a limited period.

Molecular compounds that ionise in water

Highly polar molecular compounds may form ions when dissolved in water.

Some compounds have molecules with one or more covalent bonds that are so polar they break when the compound is placed in water. Hydrogen chloride is such a compound. Hydrogen chloride (HCl) is a gas at room temperature. Chlorine is much more electronegative than hydrogen so the H—Cl covalent bond is highly polar; the molecule forms a dipole.

When hydrogen chloride is added to water, the hydrogen atom in HCl forms such a strong attraction to the oxygen atom in a water molecule that the H—Cl covalent bond breaks. The two electrons that made up the H—Cl covalent bond remain with the more electronegative Cl atom and the newly formed hydrogen ion (H^+) joins the water molecule.

Figure 13.2.9 shows that when the hydrogen ion (H^+) bonds to the water molecule, it forms a new ion known as the **hydronium ion** (H_3O^+).

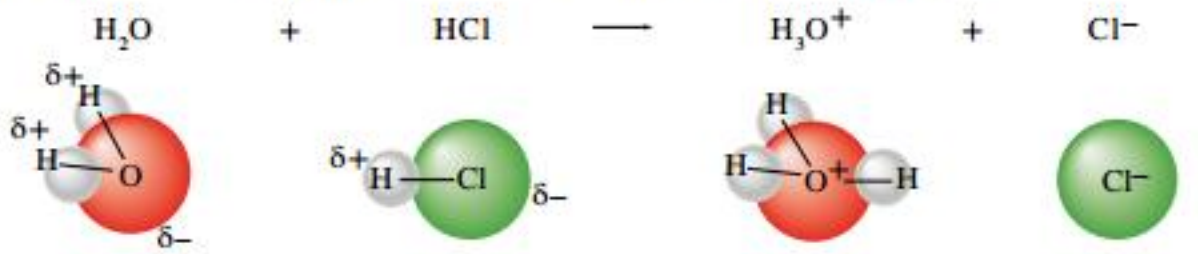


FIGURE 13.2.9 The dipole–dipole attraction between the molecules of water and hydrogen chloride leads to the breaking of the polar covalent bond between the hydrogen and chlorine atoms. New ions, hydronium and chloride, are formed in a process called ionisation.

Since the Cl atom has gained an electron, it has a negative charge, forming a chloride ion (Cl^-).

The HCl molecule is split into smaller particles, so this is a **dissociation** reaction. Dissociation means breaking apart. The HCl has also been **ionised**; that is, it has undergone a process that has produced ions (Figure 13.2.9).

Figure 13.2.10 shows how the two ions produced in the reaction of HCl with water (Cl^- and H_3O^+) become **hydrated**. The charged ions are surrounded by other polar water molecules. The polar water molecules form **ion–dipole attractions** to the Cl^- ions and to the H_3O^+ ions. The ions are described as being hydrated.

Around the chloride ions, the δ+ charges on the hydrogen atoms of surrounding water molecules are attracted to the negative charge of the chloride ion.

Around the hydronium ions, the δ– charges on the oxygen atoms of surrounding water molecules are attracted to the positive charge of the hydronium ion. (Ion–dipole attractions will be discussed again later in this module.)

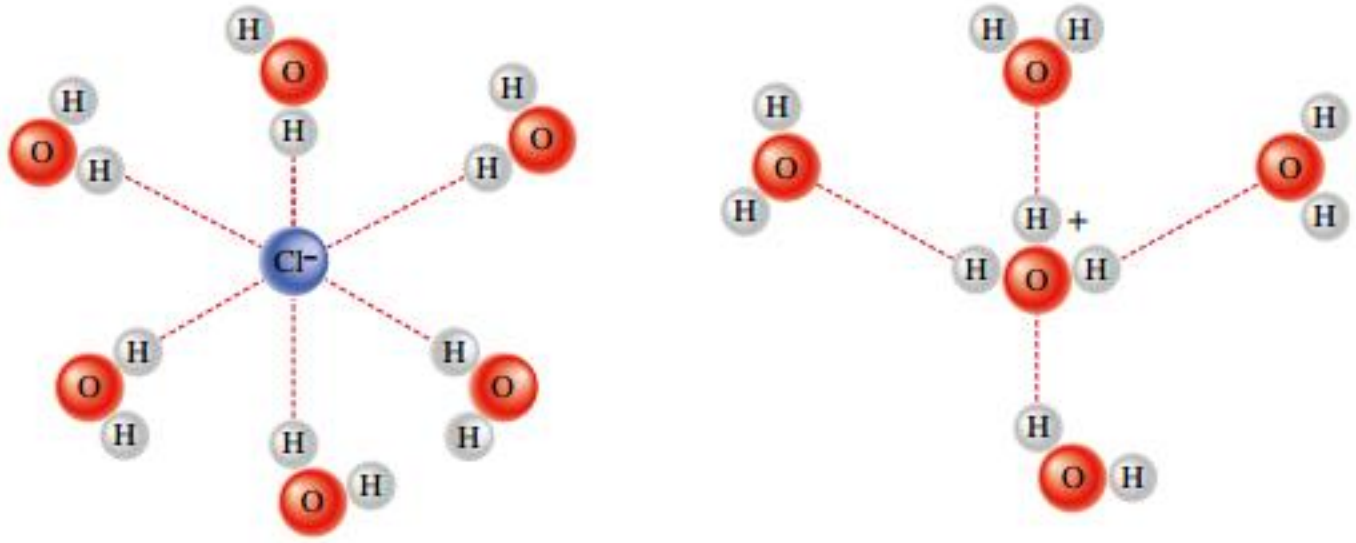


FIGURE 13.2.10 When HCl molecules ionise in water, the newly formed ions are surrounded by adjacent water molecules. The polar water molecules form ion–dipole attractions to the Cl^- ions and hydrogen bonds to the H_3O^+ ions. These bonds are represented in the diagram by dashed lines.

In summary, when hydrogen chloride dissolves in water:

- polar covalent bonds within hydrogen chloride molecules break, producing hydrogen ions (H^+) and chloride ions (Cl^-)
- a covalent bond forms between each H^+ and an H_2O molecule, forming H_3O^+ ions
- ion–dipole attractions form between the H_3O^+ and Cl^- ions and polar water molecules.

An equation can be written to represent this process:

$$HCl(g) + H_2O(l) \rightarrow H_3O^+(aq) + Cl^-(aq)$$

You should note two important points about this equation.

- Water is a reactant because there has been a rearrangement of atoms to form new substances.
- The aqueous state of the H_3O^+ and Cl^- ions tells you that they are hydrated in solution.

Other compounds that dissolve in water by ionising include the common acids nitric acid (HNO_3), sulfuric acid (H_2SO_4) and ethanoic acid (CH_3COOH).

Ammonia (NH_3) is another polar molecule that can dissolve in water. Ammonia can dissolve by either forming hydrogen bonds with water or by reacting to form the ammonium ion (NH_4^+).

Dissociation of soluble ionic compounds in water

Many ionic compounds dissolve readily in water. Sodium chloride is a typical ionic compound that exists as a solid at room temperature. In Figure 13.2.11 on page 356, you can see the arrangement of sodium cations (Na^+) and chloride anions (Cl^-) in a three-dimensional ionic lattice. The ions are held together by strong electrostatic forces between the positive and negative charges of the ions.

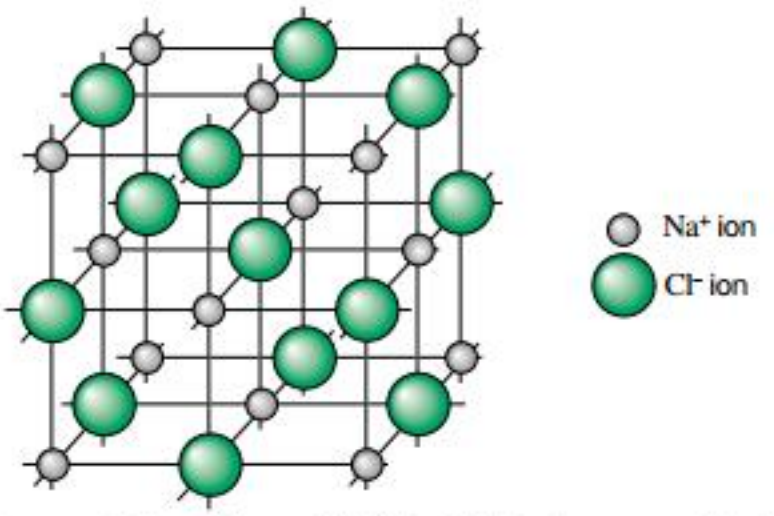


FIGURE 13.2.11 A representation of the crystal lattice of the ionic compound sodium chloride

When an ionic compound such as sodium chloride is added to water, the positive ends of the water molecules are attracted to the negatively charged chloride ions and the negative ends of the water molecules are attracted to the positively charged sodium ions (Figure 13.2.12). The attraction between an ion and a polar molecule such as water is described as an ion–dipole attraction.

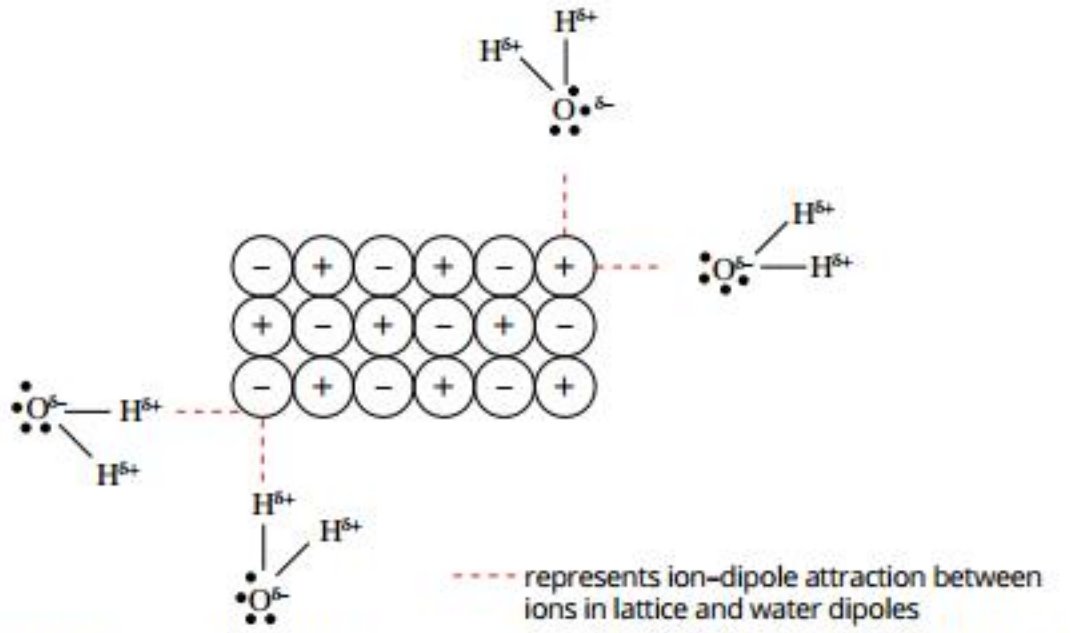


FIGURE 13.2.12 Electrostatic attraction occurs between the negative ions in a NaCl lattice and the hydrogen atoms in polar water molecules. Electrostatic attraction also occurs between the positive ions in the lattice and the oxygen atoms in water molecules.

Water molecules are in a continuous state of random motion. If the ion–dipole attractions between the ions and the water molecules are strong enough, the water molecules can pull the sodium and chloride ions on the outer part of the crystal out of the lattice and into the surrounding solution.

Sodium ions and chloride ions pulled out of the lattice become surrounded by water molecules. These ions are said to be hydrated. Water molecules are arranged around the ions as shown in Figure 13.2.13. Note the different arrangements of the water molecules around the positive and negative ions. Hydrogen atoms in the water molecules are more positive so they are orientated towards the negative chloride ion. The positive sodium ion is surrounded by the more negative oxygen atoms of the water molecules.

The process of separating positive and negative ions from a solid ionic compound to form hydrated ions when an ionic compound dissolves in water is an example of dissociation.

Although the ionic bonds within the lattice are strong, the ions can be pulled away from the lattice by the interactions of many water molecules.

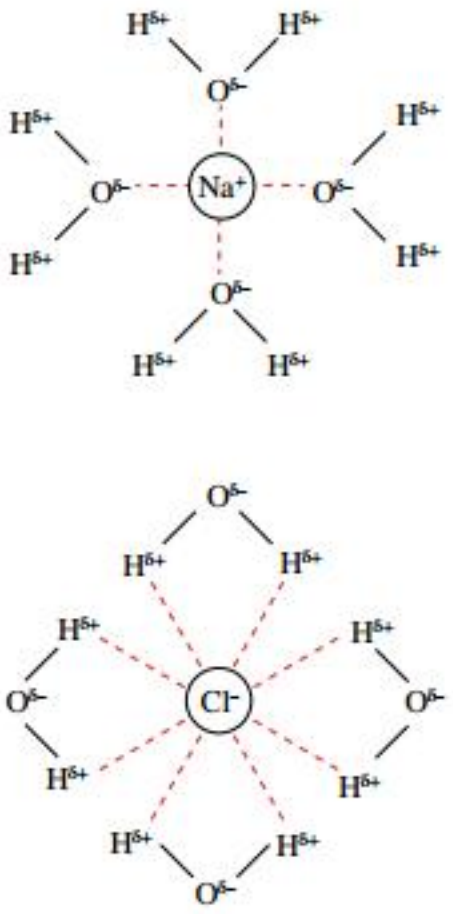


FIGURE 13.2.13 Ion–dipole attraction between the ions and adjacent water molecules form hydrated sodium and chloride ions.

In summary, when sodium chloride dissolves in water:

- ionic bonds within the sodium chloride lattice are broken
- hydrogen bonds between water molecules are broken
- ion–dipole attractions form between ions and polar water molecules.

An equation can be written to represent the dissociation process:

$$NaCl(s) \xrightarrow{H_2O(l)} Na^+(aq) + Cl^-(aq)$$

Note that the formula of water sits above the arrow. This is because there is no direct reaction between the water and the sodium chloride. No chemical change occurs; only the state symbol for sodium chloride is altered from (s) to (aq), indicating it is now dissolved in water.

It is important to note that dissociation of ionic compounds is simply freeing ions from the lattice so that they can move freely throughout the solution. This is different from ionisation of molecular compounds where new ions are formed by the reaction of the molecule with water.

Ionic substances dissolve by dissociation. Ion–dipole bonds are formed between the ions and water molecules.

Insoluble ionic compounds

Not all ionic compounds are soluble in water. For example, **limestone** ($CaCO_3$) is almost completely insoluble in water. Limestone caves such as those seen in Figure 13.2.14 are formed over a long period of time as $CaCO_3$ is dissolved and redeposited. The ionic compound $Ca_3(PO_4)_2.Ca(OH)_2$, which gives strength to bones and teeth, is also (fortunately) insoluble in water.

FIGURE 13.2.14 Limestone caves are formed by limestone (calcium carbonate) dissolving over very long periods of time. This photograph is of a limestone cave at Chillagoe, Queensland.

Insoluble ionic compounds do not dissolve in water because the forces of attraction between the ions in the lattice (ionic bonds) are much stronger than the forces of attraction between water molecules and the ions in the lattice (ion–dipole attractions).

Although substances are usually described as 'soluble' or 'insoluble', this is a generalisation. Substances that are described as 'insoluble' tend to dissolve very slightly. Those that are described as 'soluble' dissolve to varying extents.

The SNAPE rule

A handy way to remember many of the soluble salts is with the initials **SNAPE.** Salts that contain one or more of the following ions are soluble:

- **S**odium (Na^+)
- **N**itrate (NO_3^-)
- **A**mmonium (NH_4^+)
- **P**otassium (K^+)
- **E**thanoate (CH_3COO^-).

Substances are rarely ever completely 'soluble' or 'insoluble'. The solubility of substances can be considered a scale from highly soluble to almost insoluble.

Solubility tables

A **solubility table** can be used to determine whether common ionic compounds are soluble in water. Anions and cations are listed with indications of their solubility in different compounds. Table 13.2.3 on page 358 shows ionic compounds that are soluble, partially soluble, or insoluble in water.

TABLE 13.2.3 Solubility of selected compounds at 298 K

	Bromide	Carbonate	Chloride	Hydroxide	Iodide	Nitrate	Oxide	Phosphate	Sulfate
aluminium	s	–	s	i	s	s	i	i	s
ammonium	s	s	s	s	s	s	–	s	s
barium	s	i	s	s	s	s	s	i	i
calcium	s	i	s	p	s	s	p	i	p
cobalt(II)	s	i	s	i	s	s	i	i	s
copper(II)	s	–	s	i	i	s	i	i	s
iron(II)	s	i	s	i	s	s	i	i	s
iron(III)	s	–	s	i	s	s	i	i	s
lead(II)	p	i	s	i	i	s	i	i	i
lithium	s	s	s	s	s	s	s	–	s
magnesium	s	i	s	i	s	s	i	p	s
manganese(II)	s	i	s	i	s	s	i	p	s
potassium	s	s	s	s	s	s	s	s	s
silver	i	i	i	i	i	s	i	i	p
sodium	s	s	s	s	s	s	s	s	s
zinc	s	i	s	i	s	s	i	i	s

s = soluble in water (solubility greater than 10 g L^{-1})
p = partially soluble in water (solubility between 1 and 10 g L^{-1})
i = insoluble in water (solubility less than 1 g L^{-1})
– = no data

Chemistry v1.3 Formula and data book © 2021 Queensland Curriculum & Assessment Authority

Using a solubility table to predict solubility

The solubility table (Table 13.2.3) can be used to predict whether a particular ionic substance will be soluble, partially soluble or insoluble in water.

Worked example 13.2.1 shows you a systematic way of using a solubility table to determine whether an ionic compound will be soluble or insoluble in water.

Worked example 13.2.1

DETERMINING IF IONIC COMPOUNDS ARE SOLUBLE OR INSOLUBLE IN WATER

Determine if barium sulfate ($BaSO_4$) is soluble or insoluble in water. Refer to the solubility data in Table 13.2.3 to complete this question.

Thinking	Working
Identify the ions that are present in the ionic compound.	barium (Ba^{2+}) and sulfate (SO_4^{2-})
Check the solubility table to see if compounds containing the anion are usually soluble or insoluble in water.	The solubilities of compounds containing sulfate ions are listed in the last column of Table 13.2.3. Barium sulfate is insoluble in water.

➤ Try yourself 13.2.1

DETERMINING IF IONIC COMPOUNDS ARE SOLUBLE OR INSOLUBLE IN WATER

Determine if ammonium phosphate ($(NH_4)_3PO_4$) is soluble or insoluble in water. Refer to the solubility data in Table 13.2.3 to complete this question.

13.2 Review

SUMMARY

- A solution is a homogeneous mixture in which molecules or ions are evenly dispersed throughout a solvent.
- Solutions with water as the solvent are called aqueous solutions.
- A solution can form when the bonds between the solute and solvent particles are similar to or greater than the attractive forces between the solute particles and between the solvent particles.
- 'Like dissolves like' is a rule that predicts polar solutes will dissolve in polar solvents and non-polar solutes will dissolve in non-polar solvents.
- Water is a good solvent for some polar molecular compounds.
- Some polar molecular compounds dissolve by forming hydrogen bonds with water.
- Some covalent molecular compounds are so polar that they dissolve in water by ionising to form hydrated ions.
- In a hydrated ion, water molecules are attracted to the central ion by ion–dipole attractions.
- Table 13.2.4 below summarises the two ways that molecular compounds dissolve in water.

TABLE 13.2.4 The way molecular compounds dissolve in water

Type of solute	Example of solute	Bond broken in the solute	Bonds formed with water	Equation
polar covalent molecule that can hydrogen bond	ethanol, C_2H_5OH	hydrogen bonds between ethanol molecules	hydrogen bonds between ethanol and water molecules	$C_2H_5OH(l) \xrightarrow{H_2O(l)} C_2H_5OH(aq)$
polar molecules that can ionise	hydrogen chloride, HCl	covalent bond between hydrogen and chlorine atoms in the HCl molecule	covalent bond between H^+ from HCl and oxygen atom in the water molecule, forming H_3O^+ ions. H_3O^+ and Cl^- ions form ion–dipole bonds with water molecules	$HCl(g) + H_2O(l) \rightarrow H_3O^+(aq) + Cl^-(aq)$

- Soluble ionic compounds dissociate in water to form hydrated ions.
- Table 13.2.5 summarises the way soluble ionic compounds dissolve in water.
- The SNAPE rule can be used to predict the solubility of an ionic compound.
- The solubility of an ionic compound can also be found using a solubility table like Table 13.2.3 on page 358.

TABLE 13.2.5 The way ionic compounds dissolve in water

Type of solute	Example	Bond broken in the solute	Bonds formed with water	Equation
soluble ionic compounds	sodium chloride (NaCl)	ionic bonds between Na^+ and Cl^- ions	ion–dipole attractions between dissociated ions and polar water molecules	$NaCl(s) \xrightarrow{H_2O(l)} Na^+(aq) + Cl^-(aq)$

13.2 Review *continued*

KEY QUESTIONS

Describe

1 Identify each of the following components of a bottle of soft drink as solute, solvent or solution.
- **a** flavour
- **b** soft drink
- **c** water
- **d** sweetener

2 Describe how molecular substances with hydroxyl functional groups (–OH) are able to dissolve in water.

Apply

3 Explain, in terms of its structure, why vitamin C must be consumed regularly in the diet.

4 Predict if the following molecular substances are likely to be soluble or insoluble in water.
- **a** ammonia (NH_3)
- **b** oxygen gas (O_2)
- **c** hydrogen chloride (HCl)
- **d** methanol (CH_3OH)
- **e** methane (CH_4)
- **f** hydrogen fluoride (HF)
- **g** carbon dioxide (CO_2)

5 Methanol (CH_3OH) and glucose ($C_6H_{12}O_6$) form hydrogen bonds with water. They will dissolve in water without ionising. Write chemical equations to represent the dissolving process for both of these compounds.

6 With reference to the bonds that are broken and new bonds that are formed, describe how ethanol dissolves in water.

7 Hydrogen iodide (HI), like HCl, will ionise when it dissolves in water. Write a chemical equation to represent the dissolving process for this compound.

8 Write equations to show the formation of ions when the following ionic compounds dissolve in water.
- **a** potassium bromide, KBr
- **b** calcium nitrate, $Ca(NO_3)_2$
- **c** sodium sulfide, Na_2S
- **d** iron(III) chloride, $FeCl_3$
- **e** aluminium sulfate, $Al_2(SO_4)_3$

9 Redraw the representations of Na^+ and Cl^- ions below, then show the correct orientation of water molecules around hydrated sodium and chloride ions. Use a bent shape to represent the shape of water molecules.

10 Use the solubility table (Table 13.2.3 on page 358) to identify three carbonate compounds that have these characteristics:
- **a** soluble in water
- **b** insoluble in water

Analyse

11 Identify reasons for each of the following.
- **a** Concentrated deposits of nitrate compounds are only found in desert regions.
- **b** The sea is a rich source of sodium, chloride and sulfate ions.

12 Using Table 13.2.3 on page 358, predict which of the following substances will be soluble in water.
- **A** sodium carbonate
- **B** lead(II) nitrate
- **C** magnesium carbonate
- **D** zinc carbonate
- **E** silver chloride
- **F** barium sulfate

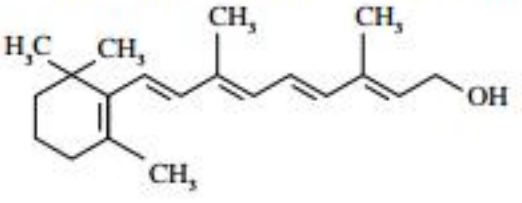
13 Sodium chloride is very soluble in water. What can be concluded about the forces present between the solute and solvent particles?

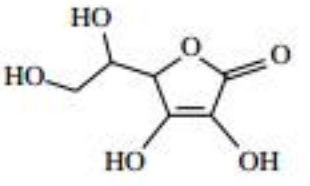
14 Fatty acids are long hydrocarbon chains with a double-bonded oxygen and hydroxyl group attached to the last carbon atom. Predict what would happen to the solubility of a fatty acid as the hydrocarbon chain length increases.

15 Compare the arrangement of water molecules around dissolved magnesium ions in water with the arrangement of chloride ions in water.

16 Methane and ammonia are similar-sized molecules. Explain, using a diagram, why methane is insoluble in water, while ammonia is highly soluble.

17 Vitamin A is a fat-soluble vitamin. Vitamin C is a water-soluble vitamin. Which of the two structures shown below (A or B) is vitamin C? Justify your answer.





13.3 Solubility

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- discriminate between unsaturated, saturated and supersaturated solutions
- identify that changes in solvent temperature can affect the solubility of solids and gases in water
- analyse solubility curves to determine the solubility of ionic compounds
- analyse data to determine the concentration of ions in aqueous solutions.

The solubility of a substance is a measure of how much of the substance will dissolve in a given amount of a solvent. For example, glucose is very soluble in water and is used by your body as a readily available energy source. Most rocks are made of minerals that are insoluble in water, but, as you saw in Module 13.2, limestone (which contains calcium carbonate) is slightly soluble and so caves form in areas of limestone rock over long periods.

In this module, you will learn how to measure the solubility of some compounds in water and how to determine solubility from a solubility curve.

DEFINITION OF SOLUBILITY

In chemistry, the term solubility has a specific meaning. It refers to the maximum amount of a solute (substance that is dissolved) that can be dissolved in a given quantity of a solvent (the common quantity often used is 100 g) at a certain temperature. Table 13.3.1 gives the solubility of some common substances in 100 g of water at 18°C.

TABLE 13.3.1 Solubility of some solutes at 18°C

Solute	Solubility (g per 100 g of water)
sugar (sucrose)	200
salt (sodium chloride)	35
limestone (calcium carbonate)	0.0013

i The solubility of a compound refers to the maximum amount of solute that can be dissolved in a given quantity of solvent at a particular temperature.

Describing degrees of saturation in solutions

There are three terms that describe the different solutions that result from dissolving solutes in solvents.

- A **saturated solution** is one in which no more solute can be dissolved at a particular temperature.
- An **unsaturated solution** contains less solute than is needed to make the solution saturated. Unsaturated solutions can dissolve more solute.
- A **supersaturated solution** is an unstable solution that contains more dissolved solute than a saturated solution. If this type of solution is disturbed, some of the solute will separate from the solvent as a solid.

Figure 13.3.1 on page 362 shows a supersaturated solution of sodium ethanoate. Supersaturated sodium ethanoate is prepared by cooling a saturated solution very carefully so that solid crystals do not form. Adding a small **seed crystal** to the supersaturated solution causes the solute to **crystallise** (form solid crystals) so that a saturated solution remains.

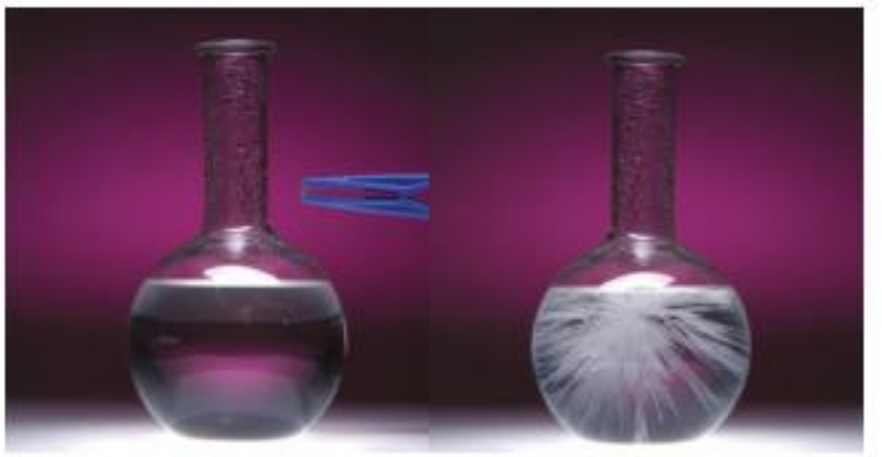


FIGURE 13.3.1 Crystals of sodium ethanoate form after a seed crystal is added to a supersaturated solution of the compound.

SOLUBILITY CURVES

The solubility of many substances changes significantly as the temperature changes. For example, you can dissolve more chocolate powder in hot milk than in cold milk. For most solids, increasing the temperature increases the solubility in a liquid. This is because at higher temperatures, both the solute and solvent have more energy to overcome the forces of attraction that hold the particles together in the solid.

The relationship between solubility and temperature can be represented by a **solubility curve** as shown in Figure 13.3.2.

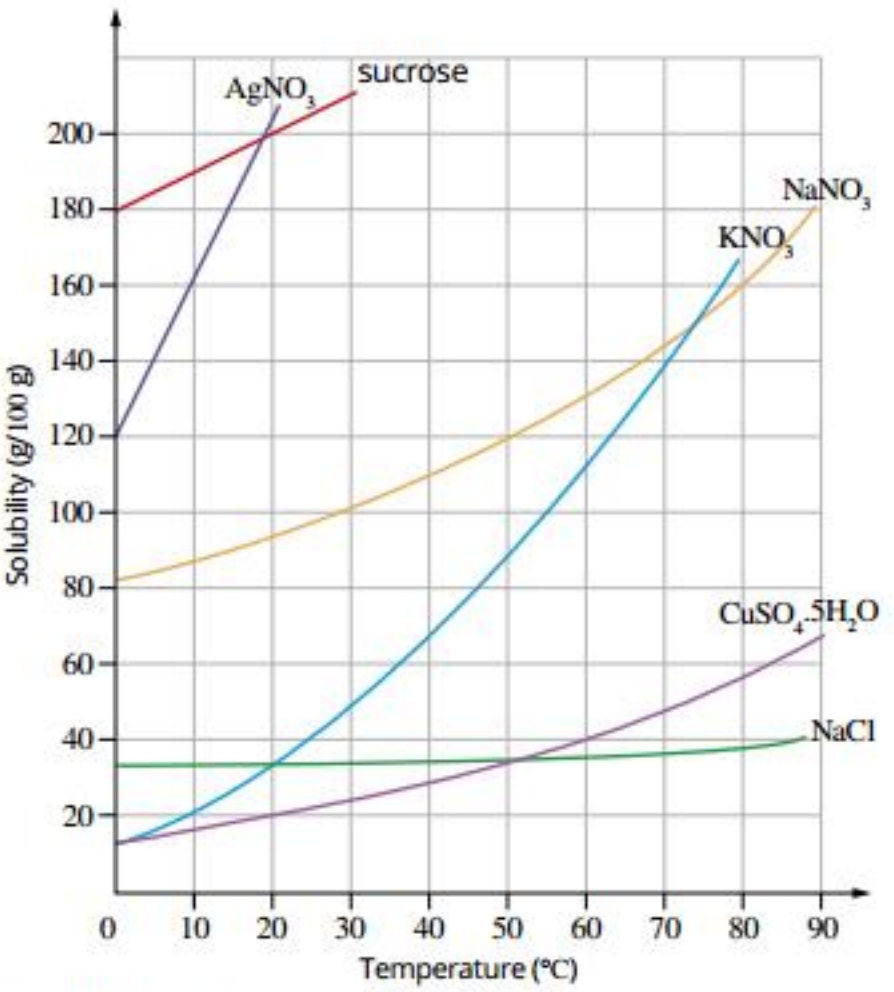


FIGURE 13.3.2 Solubility curves for some common solutes

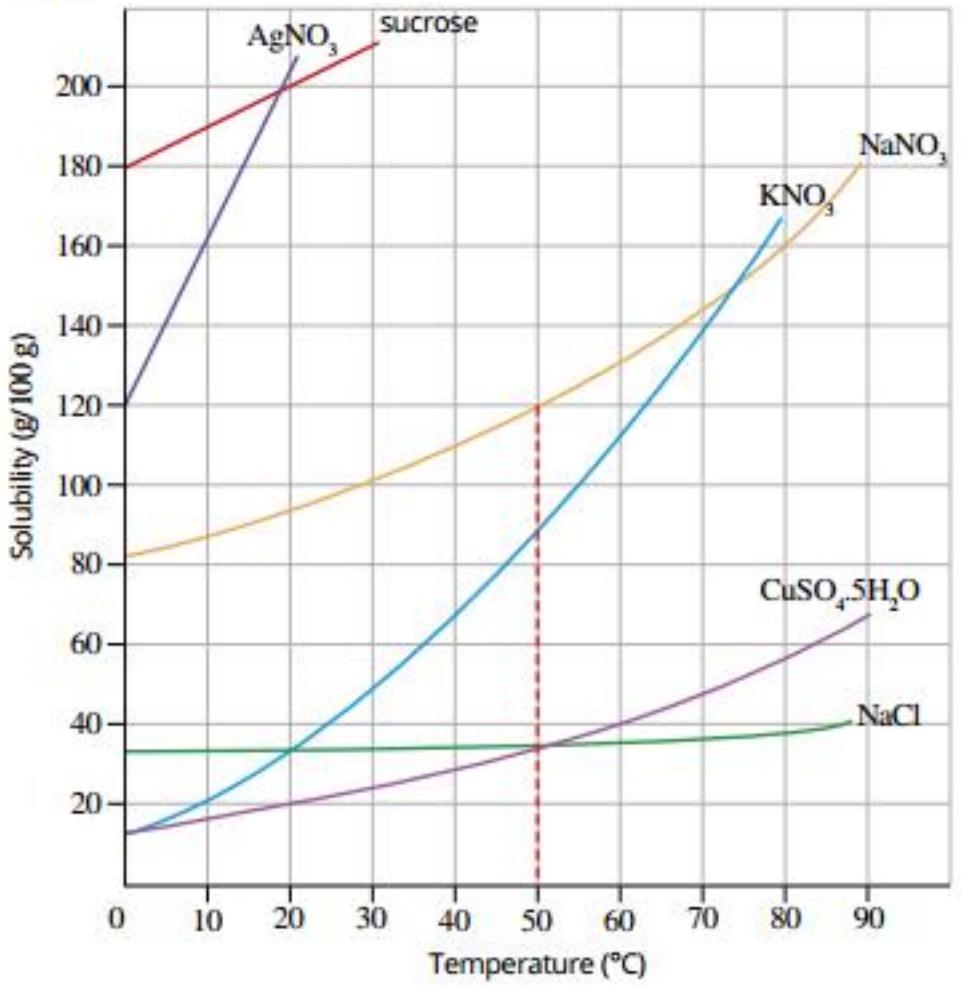
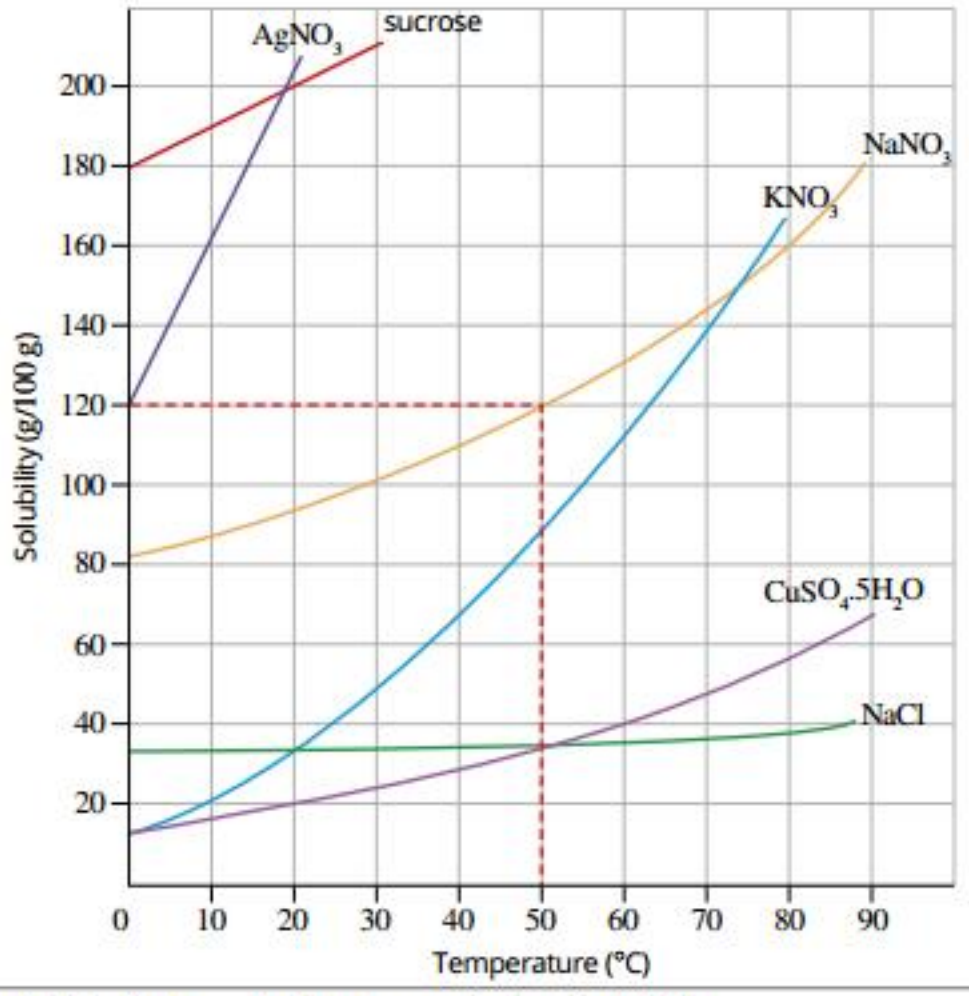
Solubility curves show the solubility of a substance as a function of temperature. For the solubility curves featured in Figure 13.3.2, note the following points.

- Each point on a curve represents the maximum amount of the solute that can be dissolved in 100 g of water at a particular temperature. Therefore, each point on the curve represents a saturated solution.
- Any point below a curve represents an unsaturated solution.
- Any point above a curve represents a supersaturated solution with a precipitate present.
- For most solids, as temperature increases, the solubility increases.

Worked example 13.3.1

SOLUBILITY CURVE CALCULATIONS

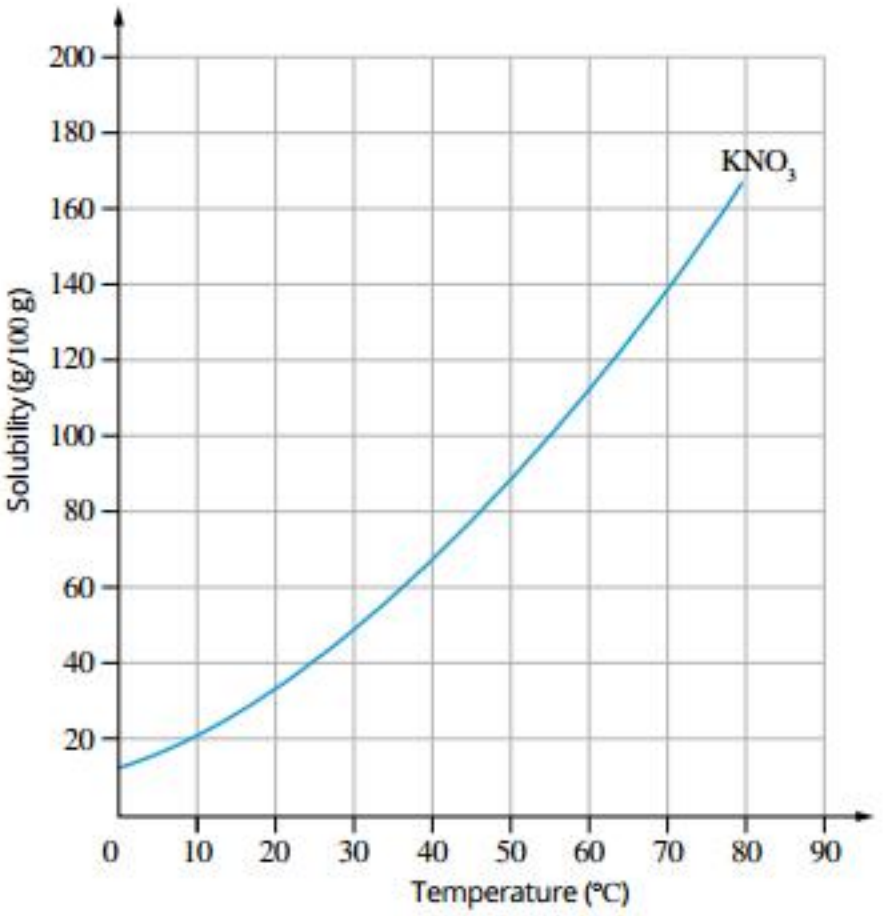
Use Figure 13.3.2 to determine how many grams of sodium nitrate ($NaNO_3$) will dissolve in 100 g of water at 50°C.

Thinking	Working
Points on a solubility curve show the maximum amount of the solute that will dissolve in 100 g water at a given temperature. Draw a vertical line from the required temperature on the horizontal axis to intersect with the appropriate solubility curve.	Draw a vertical line from 50°C on the horizontal axis to intersect with the solubility curve for $NaNO_3$. 
Draw a horizontal line from the intersection point of the vertical line drawn in the previous step. The point where this horizontal line intersects with the vertical axis will give the mass of dissolved substance.	
Read the solubility from the graph.	The horizontal line intersects with the vertical axis at 120 g. Therefore, the mass of $NaNO_3$ that will dissolve in 100 g of water at 50°C is 120 g.

➤ Try yourself 13.3.1

SOLUBILITY CURVE CALCULATIONS

Use the solubility curve below to determine how many grams of potassium nitrate (KNO_3) will dissolve in 100 g of water at 70°C.



More calculations using solubility curves

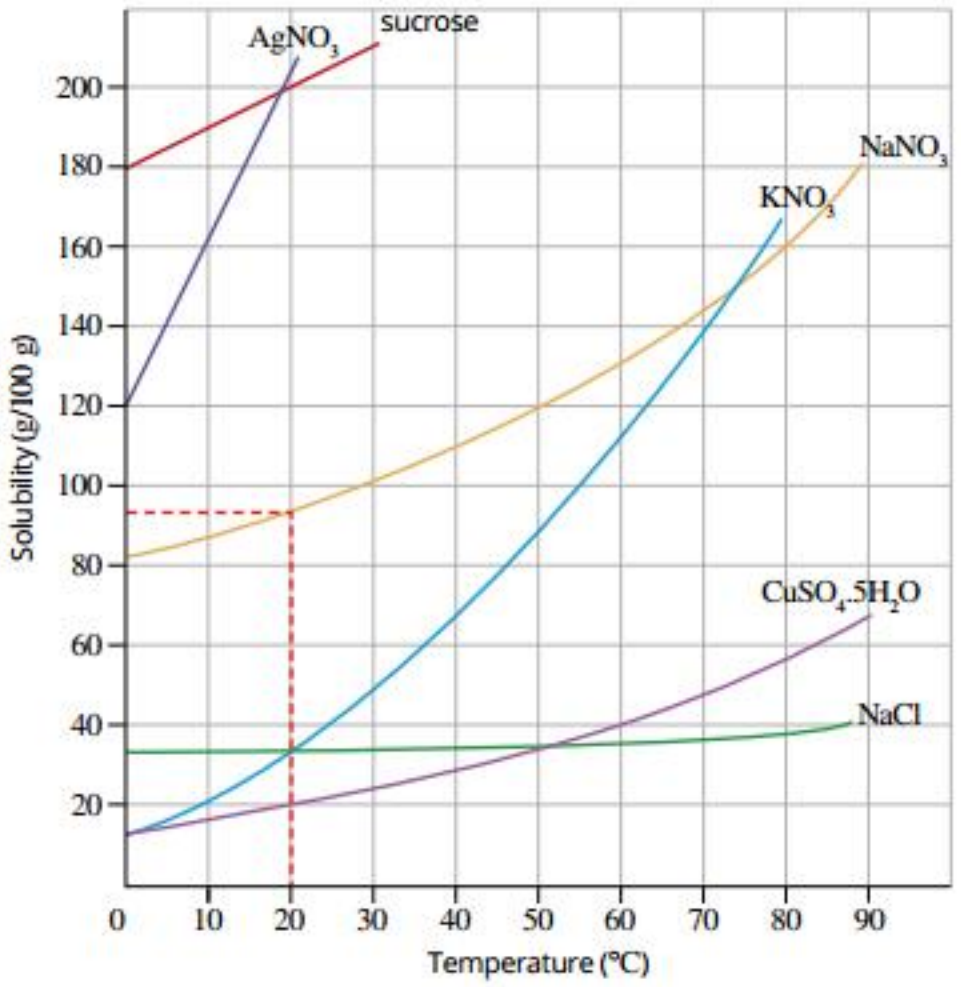
Solubility curves allow you to directly calculate the mass of a compound that will dissolve in 100g water at different temperatures. Worked example 13.3.2 shows how it is possible to use the solubility curves to calculate solubilities of compounds in quantities of water other than 100g.

Worked example 13.3.2

SOLUBILITY CURVES

An 80g sample of sodium nitrate ($NaNO_3$) is added to 200mL of H_2O at 20°C.

Use Figure 13.3.2 on page 362 to calculate how much more $NaNO_3$ must be added to make the solution saturated with $NaNO_3$ at 20°C.

Thinking	Working
Use the solubility curve to find the mass of solute in a saturated solution of 100g of H_2O at the required temperature.	Draw a line from 20°C on the horizontal axis to the solubility curve for $NaNO_3$ and find the corresponding value on the vertical axis. The value is 92g. 
Use the amount of solute that will dissolve in 100g of H_2O to find the mass of solute to make a saturated solution in the mass of H_2O for this question.	The density of water is $1.0\,g\,mL^{-1}$, so 200mL of water will weigh 200g. So twice the mass of solute can dissolve in 200g of water as in 100g. $m(NaNO_3) = 2 \times 92$ $= 184\,g$
To find out how much extra solute you need to add, find the difference between the mass of solute needed to make a saturated solution and how much has already been added.	80g of $NaNO_3$ has already been added to 200g H_2O. So the extra mass of $NaNO_3$ needed: = 184 − 80 = 104g

➤ Try yourself 13.3.2

SOLUBILITY CURVES

A 120g sample of sodium nitrate ($NaNO_3$) is added to 300mL of H_2O at 40°C.

Use Figure 13.3.2 on page 362 to calculate how much more $NaNO_3$ must be added to make the solution saturated with $NaNO_3$ at 40°C.

Weigh out several samples of different masses of potassium nitrate and record the masses.

↓

Add the samples to 20 mL (20 g) of water in separate test tubes.

↓

Heat the test tubes in a water bath and stir the contents with a thermometer until the potassium nitrate crystals dissolve.

↓

Cool the test tubes slowly with constant stirring and note the temperature (in °C) when crystals first appear. This is the temperature when the solution is just saturated with potassium nitrate. You now know what mass of potassium nitrate will form a saturated solution in 20 g of water at that temperature.

↓

Calculate what mass of potassium nitrate will saturate 100 g of water at that temperature.

↓

Plot a graph for the solubility (in g/100 g water) of potassium nitrate versus temperature (in °C).

FIGURE 13.3.3 Steps used to derive a solubility curve

Making your own solubility curve

Solubility curves can be developed relatively easily in a school laboratory. For example, a solubility curve for potassium nitrate in water can be derived in a group activity by carrying out the following steps shown in Figure 13.3.3.

SOLUBILITY OF LIQUIDS AND GASES IN WATER

It is generally true that as temperature increases, the solubility of solids in solution increases. However, the solubility of liquids in other liquids does not show clear trends in solubility as the temperature changes.

Gases generally become less soluble as the temperature increases. The graph in Figure 13.3.4 shows the solubility of different gases in water at varying temperatures.

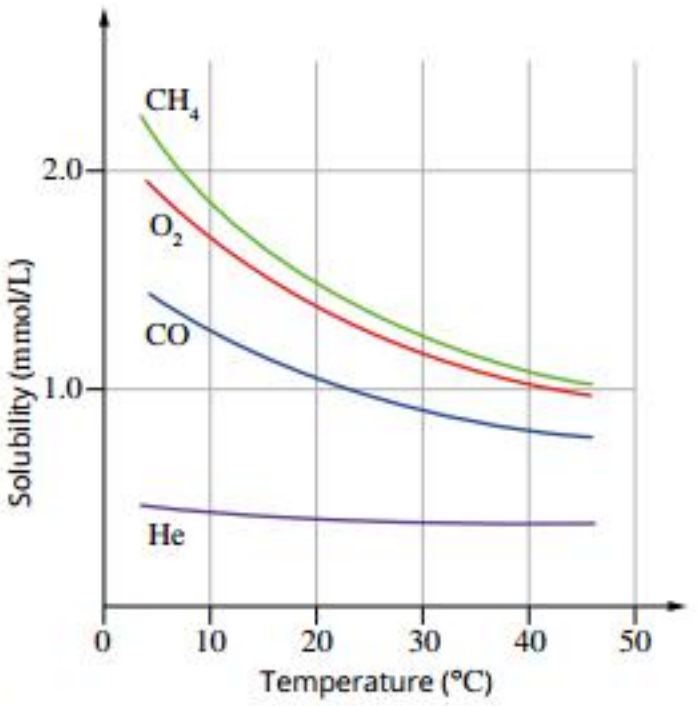


FIGURE 13.3.4 Solubility curves for some gases

Table 13.3.2 shows the solubility of some common gases in water at different temperatures. For each gas, it can be seen that as temperature increases, less gas is able to dissolve in water.

TABLE 13.3.2 Solubility of some gases in water at different temperatures

Gas	Solubility (g of gas per kg of water) at 0°C	Solubility (g of gas per kg of water) at 20°C	Solubility (g of gas per kg of water) at 60°C
oxygen	0.069	0.043	0.023
carbon dioxide	3.4	1.7	0.58
nitrogen	0.029	0.019	0.011
methane	0.040	0.023	0.011
ammonia	897	529	168

Figure 13.3.5 shows the bubbles that appear when water is first heated. The bubbles are not steam (water vapour), but bubbles of air. Some of the air that was dissolved in the water comes out of solution as the temperature increases and the gas becomes less soluble.

You may have noticed that soft drinks will go 'flat' more quickly if they are left standing in the sun on a hot day than if they are in a cold refrigerator (Figure 13.3.6). The dissolved carbon dioxide in the drink comes out of solution as the drink heats up.

FIGURE 13.3.6 Soft drinks left standing in the sun go 'flat' quickly.

FIGURE 13.3.5 Bubbles of air appear as water is heated. This is because solubility of gases decreases at higher temperatures.

The effect of temperature on the solubility of a gas can have environmental implications. If the temperature of the water in rivers, lakes and oceans increases even slightly, it will contain less dissolved oxygen. This can have serious consequences for oxygen-breathing aquatic organisms, such as the Australian Murray River cod in Figure 13.3.7.

FIGURE 13.3.7 Lowered levels of oxygen in natural waters can have serious consequences for organisms such as this Australian Murray River cod. Therefore, hot water from power stations and other industries must be cooled before it can be discharged into waterways. Even a small increase in water temperature can cause the oxygen concentration in the water to drop below levels necessary for aquatic life to survive.

13.3 Review

SUMMARY

- Solubility is a measure of how much solute will dissolve in a given amount of solvent at a specified temperature.
  - A saturated solution is one in which no more solute can be dissolved at a particular temperature.
  - An unsaturated solution contains less solute than is needed to make the solution saturated.
  - A supersaturated solution is an unstable solution that contains more dissolved solute than a saturated solution.
- Solubility curves show how the solubility of a compound changes with temperature.
- Solubility curves can be used to calculate the amount of a substance that will dissolve in a given amount of solvent at a specified temperature.
- The solubility of most solids in water increases as the temperature increases.
- As the temperature of a solution increases, the solubility of solids generally increases and the solubility of gases decreases. Liquids show no overall trend in solubility with temperature.

KEY QUESTIONS

Describe

1 Select words from the following list to complete the sentences below. Words may be used once, more than once, or not at all.
saturated solute, solution, solvent, supersaturated, temperature, unsaturated
The solubility of a substance can be measured by how much _____ will dissolve in a given quantity of _____ at a given _____. A solution that is able to dissolve more solute at a given temperature is _____. A solution in which there is more solute dissolved at a given temperature than is necessary to make the solution saturated is _____. A solution that contains the maximum amount of dissolved solute at a given temperature is _____.

2 Refer to Table 13.3.1 on page 361 to answer this question. Determine whether the following solutions are unsaturated, saturated or supersaturated.
- **a** a solution containing 35 g of sodium chloride dissolved in 100 g of water at 18°C
- **b** a solution containing 0.00045 g of calcium carbonate dissolved in 100 g of water at 18°C
- **c** a solution containing 110 g of sugar dissolved in 50 g of water at 18°C

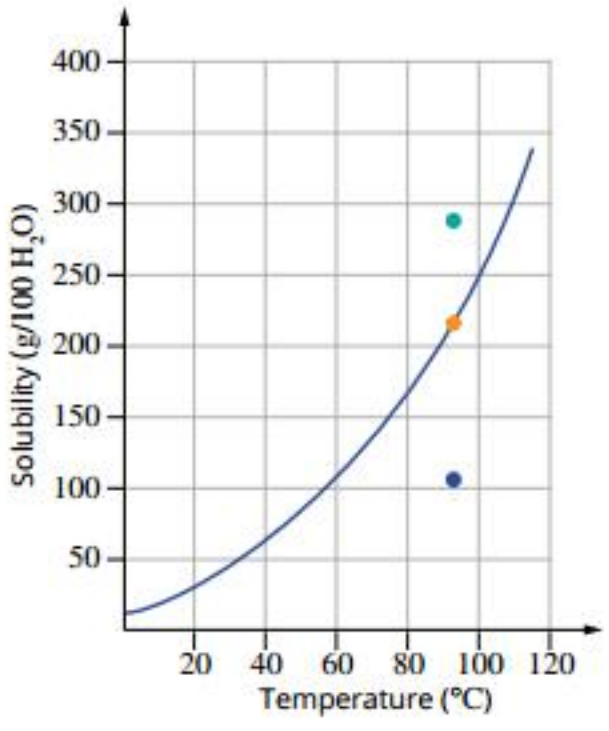
3 Refer to Figure 13.3.2 on page 362 to answer this question. How many grams of each of the following compounds would be required to make a saturated solution in 100 g of water at the temperatures shown?
- **a** $NaNO_3$ at 50°C
- **b** KNO_3 at 30°C
- **c** $CuSO_4.5H_2O$ at 60°C

4 List the information that can be determined from a solubility curve.

Apply

5 Explain the general trend seen for solubility of solutes in solution with changes in temperature.

6 Look at the graph below and determine which coloured points could correspond to saturated, unsaturated and supersaturated solutions of potassium nitrate.



7 Summarise the steps necessary to create a solubility curve for a solute in water.

Analyse

Refer to Figure 13.3.2 on page 362 to answer Questions **8** to **11**.

8 What is the maximum mass of silver nitrate ($AgNO_3$) that would dissolve at 10°C in the masses of water shown?

- **a** 100g
- **b** 20g
- **c** 300g

9 Calculate the maximum mass of solute that could dissolve in each of the following situations.

- **a** $CuSO_4.5H_2O$ in 100g of water at 60°C
- **b** $NaNO_3$ in 100g of water at 80°C
- **c** KNO_3 in 50g of water at 24°C

10 What is the mass of each solute that will dissolve in 200g of water at 30°C to form a saturated solution?

- **a** $CuSO_4.5H_2O$
- **b** $NaNO_3$
- **c** NaCl

11 Is the following statement true or false? Explain your answer.

A saturated solution of $NaNO_3$ in 200g of water at 30°C will contain less dissolved solute than a saturated solution of KNO_3 in 400g of water at 20°C.

12 A group of students carried out an experiment to derive a solubility curve for sugar (sucrose). Following the steps listed in Figure 13.3.3 on page 366, they collated the data in the table below.

Temperature (°C)	10	20	30	40	50	60	70	80
Solubility (g/100g)	191	202	217	236	260	289	324	365

Using their data, determine the following.

- **a** What type of solution will 236g of sugar form at 50°C?
- **b** What mass of sugar dissolves in 150g of water at 70°C?
- **c** What mass of water is required to dissolve 260g of sugar at 30°C?
- **d** What type of solution will form 350g of sugar and 150g water at 20°C?

13 Global climate scientists are concerned about the effect of global warming on ocean temperatures. Predict the effect of increasing the temperature of sea water on dissolved respiratory gases inhaled and exhaled by marine fauna.

14 Identify the two least soluble gases at 20°C.

15 Use Figure 13.3.4 on page 366 to determine the solubility of helium in $mmol\,L^{-1}$ at 30°C.

16 A 100g sample of sodium nitrate is dissolved in 100g of water at 40°C. Calculate how many more grams of sodium nitrate would need to be added to form a saturated solution.

13.4 Precipitation reactions

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- apply solubility rules to predict if a precipitate will be formed
- analyse data from precipitation reactions to determine the presence of specific ions in solutions
- apply ionic and chemical equations (including states) for precipitation reactions.

FIGURE 13.4.1 Undersea hydrothermal vents release superheated water containing sulfides, which form precipitates with metal ions.

In the previous module you were introduced to solubility. You also looked at the solubilities of different ions in aqueous solutions. A **precipitation reaction** occurs if ions in solution combine to form a new compound that is insoluble in water. The insoluble compound formed in such a reaction is called a **precipitate**.

Precipitation reactions occur naturally in undersea hydrothermal vents. The vents release superheated solutions containing sulfides, which then combine with metal ions to form precipitates of mineral sulfides, creating the chimney-like structures seen in Figure 13.4.1. The areas around these chimneys are biologically rich, often hosting complex communities fuelled by the chemicals dissolved in the vent fluids.

Precipitation reactions are used to remove minerals from drinking water, to remove heavy metals from wastewater and in the purification plants of reservoirs.

In this module, you will examine the process that takes place during precipitation reactions.

DEDUCING THE IDENTITY OF A PRECIPITATE

FIGURE 13.4.2 Mixing aqueous solutions of sodium chloride and silver nitrate produces a solid, called a precipitate.

When a colourless solution of silver nitrate is mixed with a colourless solution of sodium chloride, the solution turns cloudy because a very fine-powdered white solid has formed. This is shown in Figure 13.4.2. The white solid is the precipitate.

To understand what happens in the reaction between silver nitrate and sodium chloride, you need to identify the ions present in the reactant solutions and how they interact with each other.

- In the silver nitrate solution, there are dissolved silver ions (Ag^+) and nitrate ions (NO_3^-).
- In the sodium chloride solution, there are dissolved sodium ions (Na^+) and chloride ions (Cl^-).
- When one solution is added to the other, the mixture formed will contain all of the ions.

In the mixture of the two solutions, all the ions are moving around independently. As the ions move in the solution, they will collide with one another. If positive and negative ions collide, they may join together to form a new insoluble precipitate. Some of the ions have done this in the mixture of sodium chloride and silver nitrate solutions.

Two new combinations of positive and negative ions are possible:

- sodium and nitrate ions (to form sodium nitrate)
- silver and chloride ions (to form silver chloride).

You can decide which of these two compounds is the precipitate by referring to the solubility table in Table 13.2.3 (page 366). From this table we can see that, in general:

- all compounds containing a nitrate ion are soluble in water
- all compounds containing a sodium ion are soluble in water
- most compounds containing a chloride ion are soluble in water, but silver chloride is an exception.

Therefore, the precipitate shown in Figure 13.4.2 must be silver chloride.

The process for the precipitation reaction between sodium chloride and silver nitrate is shown in Figure 13.4.3. When the hydrated Ag^+ and Cl^- ions come into contact, the attraction between the ions is greater than that of the ions for the water molecules. An ionic lattice of AgCl is formed.

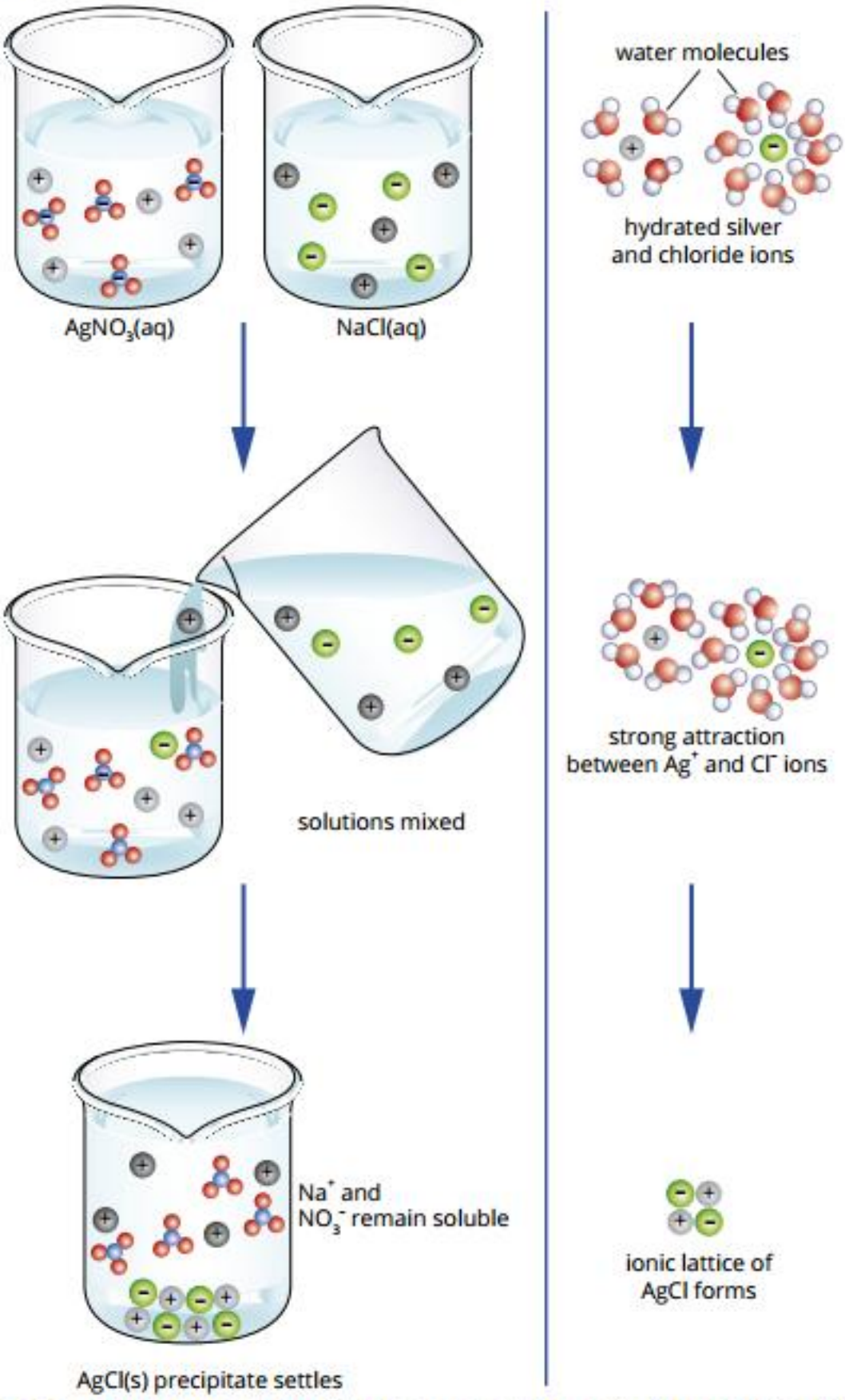


FIGURE 13.4.3 Pictorial representation of mixing aqueous solutions of sodium chloride and silver nitrate to produce a precipitate of silver chloride

There is a simple way that allows you to work out which compound will form the precipitate in a reaction between two ionic solutions.

- Write down the formula for the positive ion of one of the compounds, followed by its negative ion. Repeat the process for the second compound. For example, Ag^+, NO_3^-, Na^+, Cl^-.
- Then draw two lines. The first line joins the positive ion of the first solution to the negative ion of the second. The second line joins the negative ion of the first solution to the positive ion of the second (Figure 13.4.4).

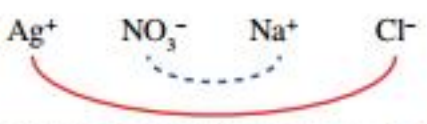


FIGURE 13.4.4 Working out which compound is the precipitate in a reaction

- Finally, use the solubility table, Table 13.2.3 on page 366, to work out which of the two combinations of ions will result in an insoluble compound. This will be the precipitate. The other ions will remain in solution.

It is important for chemists to be able to predict whether a precipitate will form in a reaction and what this precipitate will be. Worked example 13.4.1 takes you through the process of predicting the products of a precipitation reaction.

Worked example 13.4.1

PREDICTING THE PRODUCTS OF A PRECIPITATION REACTION

Determine what precipitate, if any, will be produced when solutions of potassium hydroxide and lead(II) nitrate are added together. You will need to refer to the solubility table (Table 13.2.3 on page 366) to complete this question.	
Thinking	**Working**
Identify which ions are produced by each of the ionic compounds in the mixture.	$K^+(aq)$, $OH^-(aq)$, $Pb^{2+}(aq)$ and $NO_3^-(aq)$
Identify which two new combinations of positive and negative ions are possible in the mixture of the solutions.	$K^+(aq)$ and $NO_3^-(aq)$ $Pb^{2+}(aq)$ and $OH^-(aq)$
Use the solubility table to check which, if any, of these combinations will produce an insoluble compound.	Compounds containing potassium ions are usually soluble, so potassium nitrate will not form a precipitate. Compounds containing hydroxide ions are usually insoluble, so lead(II) hydroxide will form a precipitate.

➤ Try yourself 13.4.1

PREDICTING THE PRODUCTS OF A PRECIPITATION REACTION

Determine what precipitate, if any, will be produced when solutions of sodium sulfide (Na_2S) and copper(II) nitrate ($Cu(NO_3)_2$) are added together. You will need to refer to the solubility table (Table 13.2.3 on page 366) to complete this question.

Writing equations for precipitation reactions

Now that you can identify the precipitate that forms in a reaction, the next step is to show the complete reaction by writing a chemical equation.

The reaction between silver nitrate and sodium chloride solutions can be summarised in words as:

silver nitrate solution + sodium chloride solution → silver chloride solid + sodium nitrate solution

An alternative representation is an equation that uses chemical formulas. This type of equation is called a **full equation**. The complete formulas of all the reagents and products are shown in the reaction. The state symbols for each of the species in the chemical reaction must be shown:

$$AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$$

Although 'sodium nitrate' or '$NaNO_3(aq)$' is written as a product in these equations, the sodium ions and nitrate ions are not combined with each other. You will remember from Module 13.2 that soluble ionic compounds form dissociated ions in solution and are free to move.

These ions are present at the start of the reaction and they are still there, as separate ions, at the end of the reaction. Because the ions have not been involved in forming a precipitate, they are said to be **spectator ions**.

Spectator ions do not undergo a chemical change in the reaction. In a precipitation reaction, they will always start as aqueous (aq) ions and will remain as aqueous ions after the reaction is complete.

Worked example 13.4.2 looks at the process of writing full equations for precipitation reactions and identifying spectator ions.

Worked example 13.4.2

WRITING EQUATIONS FOR PRECIPITATION REACTIONS

Write a balanced equation for the reaction between iron(III) nitrate and sodium sulfide, in which the precipitate is iron(III) sulfide. Identify the spectator ions in this reaction.	
Thinking	**Working**
Write an incomplete, unbalanced equation showing the reactants and the precipitate product. Include symbols of state.	$Fe(NO_3)_3(aq) + Na_2S(aq) \rightarrow Fe_2S_3(s)$
Add to the equation the formula of the other compound formed in the reaction.	$Fe(NO_3)_3(aq) + Na_2S(aq) \rightarrow Fe_2S_3(s) + NaNO_3(aq)$
Balance the equation.	$2Fe(NO_3)_3(aq) + 3Na_2S(aq) \rightarrow Fe_2S_3(s) + 6NaNO_3(aq)$
Write the formulas of the ions that do not form a precipitate in the reaction. These are the spectator ions.	$Na^+(aq)$ and $NO_3^-(aq)$ are spectator ions.

➤ Try yourself 13.4.2

WRITING EQUATIONS FOR PRECIPITATION REACTIONS

Write a balanced equation for the reaction between copper(II) sulfate and sodium hydroxide, in which the precipitate is copper(II) hydroxide. Identify the spectator ions in this reaction.

Writing ionic equations for precipitation reactions

The essential feature of the reaction between silver nitrate and sodium chloride is the combination of silver ions and chloride ions to form a precipitate. This reaction can be summarised in an **ionic equation**:

$$Ag^+(aq) + Cl^-(aq) \rightarrow AgCl(s)$$

Note that spectator ions are not included in an ionic equation. Only the species that change are included.

An ionic equation can be thought of as a full equation with the spectator ions removed. So full and ionic equations for the reaction between silver nitrate and sodium chloride solutions are:

Full equation: $AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$

Ionic equation: $Ag^+(aq) + Cl^-(aq) \rightarrow AgCl(s)$

A simple way to write an ionic equation for a precipitation reaction is shown in the following example of the reactions between solutions of aluminium nitrate and sodium sulfide. The full equation for the precipitation reaction is:

$$2Al(NO_3)_3(aq) + 3Na_2S(aq) \rightarrow Al_2S_3(s) + 6NaNO_3(aq)$$

To write an ionic equation:

- Write down the formula of the precipitate on the right-hand side of the page. Include a symbol of state. Place an arrow to the left of it.

$$\rightarrow Al_2S_3(s)$$

- To the left of this formula, add the formulas of the ions that form the precipitate, in the ratio shown by the formula of the precipitate. Include state symbols.

$$2Al^{3+}(aq) + 3S^{2-}(aq) \rightarrow Al_2S_3(s)$$

- Check that the equation is balanced.

Worked example 13.4.3 looks at the process of writing ionic equations for precipitation reactions.

Worked example 13.4.3

WRITING IONIC EQUATIONS FOR PRECIPITATION REACTIONS

Write a balanced ionic equation for the reaction between silver nitrate and potassium carbonate.	
Thinking	**Working**
Write an incomplete, unbalanced equation showing the reactants and the precipitate product. Include symbols of state.	$AgNO_3(aq) + K_2CO_3(aq) \rightarrow Ag_2CO_3(s) + KNO_3(aq)$
Write down the formula for the precipitate on the right-hand side of the page and place an arrow to the left of it.	$\rightarrow Ag_2CO_3(s)$
Add the formulas of the ions that form the precipitate, in the ratio shown by the formula of the precipitate.	$2Ag^+ + CO_3^{2-} \rightarrow Ag_2CO_3(s)$
Add states to the reactant side of the equation.	$2Ag^+(aq) + CO_3^{2-}(aq) \rightarrow Ag_2CO_3(s)$

➤ Try yourself 13.4.3

WRITING IONIC EQUATIONS FOR PRECIPITATION REACTIONS

Write a balanced ionic equation for the reaction between magnesium chloride and sodium sulfide.

13.4 Review

SUMMARY

- A precipitation reaction occurs when two solutions of compounds are mixed and a solid product is formed. The solid product is called a precipitate.
- Solubility tables can be used to predict which compound, if any, will precipitate in a reaction.
- Ions that are not directly involved in the formation of the precipitate during a precipitation reaction are called spectator ions.
- Full and ionic equations can be written for precipitation reactions. Both equation types use chemical formulas and include state symbols (s), (l), (g) and (aq).
- Ionic equations do not include spectator ions.

KEY QUESTIONS

Describe

1 Use the solubility table, Table 13.2.3 on page 366, to identify the precipitate formed, if any, when the following solutions are mixed.

a silver nitrate and potassium carbonate
b potassium hydroxide and lead(II) nitrate
c magnesium chloride and sodium sulfide
d sodium chloride and iron(II) sulfate

2 **a** Write the formula of the precipitate formed, if any, when the following solutions are mixed.

i $Ca(NO_3)_2$ and K_2CO_3
ii $MgSO_4$ and $Cu(NO_3)_2$
iii Na_2S and $MgSO_4$
iv $FeCl_2$ and NH_4OH
v Na_3PO_4 and $AgNO_3$

b Write the formulas of any spectator ions in the questions in part **a**.

3 **a** Name the precipitate formed when aqueous solutions of the following compounds are mixed.

i K_2S and $MgCl_2$
ii $CuCl_2$ and $AgNO_3$
iii KOH and $AlCl_3$
iv $MgSO_4$ and NaOH

b Write a balanced full chemical equation for each reaction.

Apply

4 Represent the process of precipitation with a diagram similar to that shown in Figure 13.4.4 on page 371 for the reaction between lead(II) nitrate and sodium hydroxide.

5 Show, using a balanced full chemical equation, how two solutions can produce a solid precipitate using barium chloride and sodium sulfate.

Analyse

6 For each of the following combinations of solutions, represent the reactions that occur by:

i a full equation
ii an ionic equation

a $NH_4Cl + AgNO_3$
b $Cu(NO_3)_2 + K_2CO_3$
c $Pb(CH_3COO)_2 + Na_2SO_4$

7 For each of the parts **a–c** in Question **6**, identify the spectator ions.

8 Distinguish between a full chemical equation and an ionic equation using the precipitation reaction between ammonium sulfate and barium chloride as an example.

9 Identify whether each of the following ions, when combined with Fe^{2+}, would form a precipitate.

a SO_4^{2-}
b PO_4^{3-}
c Br^-

10 Using your knowledge of solubility, infer which positive ions are most likely to act as spectator ions in a precipitation reaction.

11 Aqueous solutions of potassium sulfate, barium ethanoate and magnesium nitrate were added to a beaker and a precipitate formed.

a Name the precipitate.
b Write a full equation for the reaction.
c Write an ionic equation for the reaction.

12 Describe how you could obtain a pure sample of solid sodium chloride using solutions of sodium sulfate and barium chloride.

13.5 Concentration of solutes in solution

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- discriminate between the terms solute, solvent, solution and concentration
- apply the mole concept to calculate the molar concentration, moles of solute and volume of solution of different solutions using multiple units
- calculate the concentration of diluted solutions
- conduct a number of calculations to convert between the different units of concentration.

The concentration of a solution describes the relative amount of solute and solvent present in the solution. A solution in which the ratio of solute to solvent is high is said to be concentrated. Cordial that has not had any water added to it is an example of a **concentrated solution**. A solution in which the ratio of solute to solvent is low is said to be a **dilute solution**. A quarter of a teaspoon of sugar dissolved in a litre of water will produce a dilute solution that tastes slightly sweet.

'Concentrated' and 'dilute' are general terms. However, sometimes you need to know the actual concentration of a solution—the exact ratio of solute to solvent. The use of exact solution concentrations is important in the prescription of medicines, chemical manufacturing and chemical analysis.

UNITS OF CONCENTRATION

Chemists use different measures of concentration depending on the situation. The most common measures describe the amount of solute in a given amount of solution.

Here are some examples of units of concentration.

- grams per litre, $g\,L^{-1}$
- moles per litre, $mol\,L^{-1}$
- parts per million (ppm)
- percentage by mass or percentage by volume.

When very small quantities of solute, such as chemicals in the environment, are dissolved to form a solution, the concentration can be measured in parts per million. For example, the concentration of mercury in fish is usually expressed in parts per million. You might have noticed symbols such as %(w/v) or %(v/v) on the labels of some foods, drinks and pharmaceuticals. These symbols represent the mass or volume of solute as a percentage of the solution. For example, the label on a bottle of wine might display 14.5% alc./vol. This means the wine contains 14.5 mL of alcohol (ethanol) in 100 mL of wine.

Concentration units have two parts. The first part provides information about how much solute is present. The second part provides information about how much solution is present.

Units of concentration measured in this way have two parts.

- The first part gives information about how much solute there is.
- The second part gives information about how much solution there is.

For example, if a solution contains sodium chloride (NaCl) with a concentration of $17\,g\,L^{-1}$, then (first part) 17 g of NaCl is dissolved in every (second part) 1 L of the solution.

You will now look at how to perform calculations of concentration using different units.

Concentration in grams per litre (gL^{-1})

The concentration of a solution in grams per litre (gL^{-1}) indicates the mass, in grams, of solute dissolved in 1 litre of the solution. For example, if the concentration of sodium chloride in sea water is $20\,gL^{-1}$, this means that in 1 L of sea water there is 20 g of sodium chloride. A formula used to calculate the concentration in gL^{-1} is:

$$\text{concentration } (gL^{-1}) = \frac{\text{mass of solute (in g)}}{\text{volume of solution (in L)}}$$

Worked example 13.5.1

CALCULATING CONCENTRATION IN gL^{-1} (GRAMS PER LITRE)

Calculate the concentration, in gL^{-1}, of a solution containing 8.00 g of sodium chloride in 500 mL of solution.	
Thinking	**Working**
Change the volume of solution so it is expressed in litres.	$500\,mL = \frac{500}{1000} = 0.500\,L$
Calculate the concentration in gL^{-1}.	$c = \frac{\text{mass of solute (in g)}}{\text{volume of solution (in L)}}$ $= \frac{8.00\,g}{0.500\,L}$ $= 16.0\,gL^{-1}$

➤ Try yourself 13.5.1

CALCULATING CONCENTRATION IN gL^{-1} (GRAMS PER LITRE)

Calculate the concentration, in gL^{-1}, of a solution containing 5.00 g of glucose in 250 mL of solution.

Concentration in milligrams per litre (mgL^{-1})

If, for example, the concentration of cadmium in a sample of wastewater was $5\,mgL^{-1}$, this means that in 1 litre of the wastewater there will be 5 mg of cadmium. Concentrations in mgL^{-1} may be calculated using the formula:

$$\text{concentration } (mgL^{-1}) = \frac{\text{mass of solute (in mg)}}{\text{volume of solution (in L)}}$$

A concentration of solution measured in units of ppm has the same value as concentration measured in $mgkg^{-1}$. Since 1 litre of solution has a mass of almost exactly 1 kilogram, then a concentration measured in mgL^{-1} will also have the same value in units of ppm, i.e.

$$1\,ppm = 1\,mgkg^{-1} = 1\,mgL^{-1}$$

For example, the concentration, in mgL^{-1} and ppm, of 2.0 L of a sugar solution containing 0.050 g of sugar can be calculated as follows:

$$0.050\,g \text{ of sugar} = 50\,mg$$

$$\text{concentration } (mgL^{-1}) = \frac{50}{2.0}$$

$$= 25\,mgL^{-1}$$

$$= 25\,ppm$$

i Concentrations in mgL^{-1} and in ppm are equivalent.

Concentration in parts per million (ppm)

When very small quantities of solute are dissolved to form a solution, the concentration is often measured in **parts per million (ppm)**. For example, the concentration of mercury in fish that is suitable for consumption is usually expressed in parts per million. The maximum concentration allowed for sale in Australia is 1 ppm (Figure 13.5.1).

FIGURE 13.5.1 Fish sold in Australia must have no more than 1 ppm of mercury (Australia New Zealand Food Standards Code).

In simple terms, the concentration in parts per million can be thought of as the mass in grams of solute dissolved in 1 000 000 g of solution. This can also be expressed as the mass in milligrams of solute dissolved in 1 kg of solution, because there are 1 million milligrams in a kilogram.

For example, a solution of sodium chloride that has a concentration of 154 ppm contains 154 mg of sodium chloride dissolved in 1 kg of solution. A formula used to calculate the concentration of a solution in ppm is:

$$\text{concentration (ppm)} = \frac{\text{mass of solute (in mg)}}{\text{mass of solution (in kg)}}$$

Worked example 13.5.2

CALCULATING CONCENTRATION IN PARTS PER MILLION (PPM)

A saturated solution of calcium carbonate was found to contain 0.0198 g of calcium carbonate dissolved in 2000 g of solution. Calculate the concentration, in ppm, of calcium carbonate in the saturated solution.

Thinking	Working
Calculate the mass of solute in mg. Remember: mass (in mg) = mass (in g) × 1000	mass of solute (calcium carbonate) in mg = 0.0198 × 1000 = 19.8 mg
Calculate the mass of solution in kg. Remember: $\text{mass (in kg)} = \frac{\text{mass (in g)}}{1000}$	$\text{mass of solution in kg} = \frac{2000}{1000}$ = 2.000 kg
Calculate the concentration of the solution in mg kg^{-1}. This is the same as concentration in ppm.	concentration of calcium carbonate in ppm $= \frac{\text{mass of solute (in mg)}}{\text{mass of solution (in kg)}}$ $= \frac{19.8}{2.000}$ $= 9.90\ \text{mg kg}^{-1}$ = 9.90 ppm

➤ Try yourself 13.5.2

CALCULATING CONCENTRATION IN PARTS PER MILLION (PPM)

A sample of tap water was found to contain 0.0537 g of NaCl per 250.0 g of solution. Calculate the concentration of NaCl in parts per million (ppm).

FIGURE 13.5.2 Consumer products from hardware stores and supermarkets show a wide range of concentration units on their labels.

Other units of concentration

You might have noticed symbols such as m/m, v/v or m/v on the labels of some foods, drinks and pharmaceuticals. These symbols represent other concentration units based on masses and volumes of solutes and solutions. These are useful in practical situations because people are familiar with these quantities (Figure 13.5.2).

Percentage by mass (m/m)

Percentage by mass describes the mass of solute, measured in grams, present in 100 g of the solution.

Normal saline solution for washing contact lenses has a concentration of 0.9%(w/w). This can also be written as 0.9%(m/m). The abbreviation w/w indicates that the percentage is based on the weights or, more correctly, masses of both solute and solution. A concentration of 0.9% indicates that there is 0.9 g of sodium chloride dissolved in 100 g of solution.

Percentage by volume (v/v)

The abbreviation v/v indicates that the percentage is based on volumes of both solute and solution. The same units must be used to record both volumes. Percentage by volume is a more convenient unit to use than w/w when the solute is a liquid.

Just like percentage by mass, percentage by volume is frequently expressed as volume per 100 mL of solution. For example, the wine label in Figure 13.5.3 shows 13.5% alc./vol. This means the wine contains 13.5% alcohol (ethanol) by volume (13.5%(v/v)). There will be 13.5 mL of alcohol in 100 mL of the wine.

TARRAWARRA
ESTATE
2023 PINOT NOIR
YARRA VALLEY
SLOW MOVING WATER
2023 PINOT NOIR
An expression of our Estate vineyard. Lively light purple hue. Raspberry, violets and red cherry aromatics. Elegant, graceful and pure to the core.
TARRAWARRA
311 HEALESVILLE - YARRA GLEN ROAD YARRA GLEN VIC 3775 AUSTRALIA
PREGNANCY WARNING
Alcohol can cause lifelong harm to your baby
13.5% ALC/VOL
8.0 STANDARD DRINKS APPROX
CONTAINS SULPHITES
TARRAWARRA.COM.AU
WINE OF AUSTRALIA
750ML
9 083520 900707

FIGURE 13.5.3 The label from a bottle of Yarra Valley wine shows the alcohol concentration in units of %(v/v).

For example, a 200 mL glass of champagne contains 27 mL of alcohol. The concentration as %(v/v) of alcohol in this solution can be calculated as follows:

$$\text{concentration (\% (v/v))} = \frac{\text{volume of solute (in mL)}}{\text{volume of solution (in mL)}} \times 100\%$$

$$= \frac{27}{100} \times 100\%$$

$$= 13.5\%\text{(v/v)}$$

Percentage mass/volume (m/v)

Percentage mass/volume describes the mass of solute, measured in grams, present in 100 mL of the solution.

For example, if a solution of plant food contains a particular potassium compound at a concentration of 3%(m/v), this indicates that there is 3 g of potassium in 100 mL of solution.

CALCULATING CONCENTRATION IN MOLES PER LITRE

Units of concentration such as gL^{-1}, %(m/v) and %(v/v) are commonly used on the labels of consumer products found in supermarkets, pharmacies and hardware stores. These units are rarely used in school chemistry laboratories and in chemistry research laboratories in general. This is because quantitative calculations using these units can be inconvenient and lengthy. The unit favoured by chemists is $molL^{-1}$. However, unless people have had some training in chemistry, they will not have an understanding of the chemical terms 'mole' and '$molL^{-1}$'. It is unlikely that you will see this unit used on product shelves in your supermarket.

Concentrations expressed in moles per litre ($molL^{-1}$) allow chemists to compare the number of moles of atoms, molecules or ions present in a given volume of solution.

For example, a 0.1 $molL^{-1}$ solution of hydrochloric acid would contain 0.1 moles of HCl in 1 L of the solution. (A bottle of HCl of this concentration is shown in Figure 13.5.4.)

FIGURE 13.5.4 These bottles contain solutions with concentrations shown in units of M ($molL^{-1}$).

The concentration, in mol L^{-1}, of a solution can be calculated as follows:

$$\text{concentration (mol L}^{-1}) = \frac{\text{amount of solute (in mol)}}{\text{amount of solution (in L)}}$$

This can be written using variables:

$$c = \frac{n}{V}$$

where c is the concentration (mol L^{-1}), n is the amount (mol) and V is the volume (L).

The concentration of a solution in moles per litre is often referred to as the **molarity**, or molar concentration, of the solution, and is given the unit M.

$$\text{molarity} = \frac{\text{moles of solute } (n)}{\text{volume of solution } (V)}$$

$$M = \frac{n}{V}$$

A solution containing 1 mole of solute dissolved in 1 litre of solution can therefore be described in several different ways. You can say that the solution:

- has a concentration of 1 mole per litre
- has a concentration of 1 mol L^{-1}
- is 1 molar
- is 1 M
- has a molarity of 1 M.

Worked example 13.5.3

CALCULATING MOLAR CONCENTRATIONS (MOLARITY)

Calculate the molar concentration of a solution that contains 0.105 mol of potassium nitrate dissolved in 200 mL of solution.

Thinking	Working
Convert the given volume to litres.	$V(KNO_3) = \frac{200}{1000}$ $= 0.200\,L$
Calculate the molar concentration using the formula: $c = \frac{n}{V}$	$c(KNO_3) = \frac{n}{V}$ $= \frac{0.105}{0.200}$ $= 0.525\,\text{mol L}^{-1}$ or $0.525\,M$

➤ **Try yourself 13.5.3**

CALCULATING MOLAR CONCENTRATIONS (MOLARITY)

Calculate the molar concentration of a solution that contains 0.24 mol of glucose dissolved in 500 mL of solution.

Calculating molarity given the mass of solute

Sometimes you will know the mass of a solute and volume of solution and want to calculate the molarity. Two main calculations are involved.

1 Calculate the number of moles of solute from its mass.
2 Calculate the concentration using the number of moles and the volume (in litres).

Worked example 13.5.4

CALCULATING MOLARITY GIVEN THE MASS OF SOLUTE

Calculate the concentration, in mol L^{-1}, of a solution that contains 16.8 mg of silver nitrate ($AgNO_3$) dissolved in 150 mL of solution.	
Thinking	**Working**
Convert the volume to litres.	$V(AgNO_3) = \frac{150}{1000}$ $= 0.150\,L$
Convert the mass to grams.	$m(AgNO_3) = \frac{16.8}{1000}$ $= 0.0168\,g$
Calculate the molar mass of the solute. To do this, add up the atomic masses of all the atoms in the compound.	$M(AgNO_3) = 107.87 + 14.01 + (3 \times 16.00)$ $= 169.88\,g\,mol^{-1}$
Calculate the number of moles of solute using the formula: $n = \frac{m}{M}$	$n(AgNO_3) = \frac{m}{M}$ $= \frac{0.0168}{169.9}$ $= 9.89 \times 10^{-5}\,mol$
Calculate the molar concentration using the formula: $c = \frac{n}{V}$	$c(AgNO_3) = \frac{n}{V}$ $= \frac{9.89 \times 10^{-5}}{0.150}$ $= 6.59 \times 10^{-4}\,mol\,L^{-1}$ or $6.59 \times 10^{-4}\,M$

> **The symbol *M* was used earlier to represent molar mass. Take care not to confuse the two different uses: *M* is a quantity symbol; M is a unit symbol and is equivalent to mol L^{-1}.**

➤ Try yourself 13.5.4

CALCULATING MOLARITY GIVEN THE MASS OF SOLUTE

Calculate the concentration, in mol L^{-1}, of a solution that contains 4000 mg of ethanoic acid (CH_3COOH) dissolved in 100 mL of solution.

Calculating the number of moles of solute in a solution

The formula used to calculate the molarity of a solution is $c = \frac{n}{V}$. If you rearrange the formula, you can use it to calculate the number of moles of solute in a solution of given concentration and volume:

$$n = c \times V$$

where n is the amount (mol), c is the concentration (mol L^{-1}) and V is the volume (L).

Worked example 13.5.5

CALCULATING THE NUMBER OF MOLES OF SOLUTE IN A SOLUTION

Calculate the number of moles of ammonia (NH_3) in 25.0 mL of a 0.3277 M ammonia solution.	
Thinking	**Working**
Convert the given volume to litres.	$V(NH_3) = \frac{25.0}{1000}$ $= 0.0250\,L$
Calculate the number of moles of the compound, using the formula: $n = c \times V$	$n(NH_3) = c \times V$ $= 0.3277 \times 0.0250$ $= 8.19 \times 10^{-3}\,mol$

➤ Try yourself 13.5.5

CALCULATING THE NUMBER OF MOLES OF SOLUTE IN A SOLUTION

Calculate the number of moles of potassium permanganate ($KMnO_4$) in 100 mL of a 0.0250 M solution of the compound.

DILUTION

FIGURE 13.5.5 Pesticide solutions used in aerial spraying are prepared by diluting a concentrated solution of the pesticide compound.

Many commercially available domestic and industrial products come in the form of concentrated solutions. Examples are pesticides (Figure 13.5.5), fertilisers, detergents, fruit juices, acids and other chemicals. A major reason for using concentrates is to save on transportation costs. Diluted solutions contain a lot of water and that extra mass has to be transported, which increases costs. It is also more convenient to buy concentrated products and dilute with water at home or in the workplace.

Everyday examples of dilution are:

- adding water to cordial
- a laboratory technician making a 1 M solution of hydrochloric acid from a bottle of concentrated hydrochloric acid
- a home gardener diluting fertiliser concentrate to spray on the lawn
- a farmer diluting weedkiller concentrate to spray on a wheat crop
- an assistant in a commercial kitchen diluting concentrated detergent solution before using it to wash dishes.

In this module, you will learn how to calculate the concentrations of solutions after they have been diluted.

Calculating concentrations when solutions are diluted

The process of adding more solvent to a solution is known as **dilution**. When a solution is diluted, its concentration is decreased.

For example, if 50 mL of water is added to 50 mL of 0.10 mol L^{-1} sugar solution, the amount of sugar remains unchanged but the volume of the solution in which it is dissolved doubles. As Figure 13.5.6 shows, this means the sugar molecules are spread further apart during the dilution process, and so the concentration of the sugar solution is decreased (it will become 0.050 mol L^{-1} in this instance).

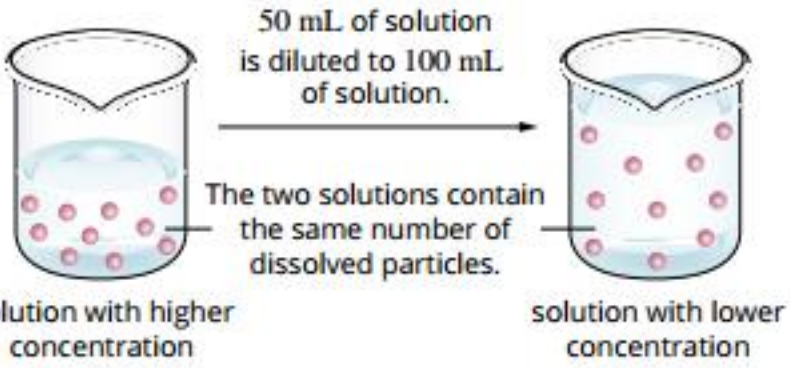


FIGURE 13.5.6 Dilution does not change the number of solute particles but the concentration of the solute decreases.

It is important to recognise that diluting a solution (by adding more solvent) does not change the number of moles of the solute present.

Suppose you had V_1 litres of a solution and the concentration was c_1 mol L^{-1}. The number of moles of the solute is given by:

$$n_1 = c_1 \times V_1$$

Suppose water was added to make a new volume, V_2, which changes the concentration to c_2. The number of moles of the solute, n_2, in this diluted solution is given by:

$$n_2 = c_2 \times V_2$$

Since the number of moles of solute has not changed, $n_1 = n_2$; therefore:

$$c_1V_1 = c_2V_2$$

This formula is useful when solving problems involving diluted solutions. (Note that this formula can also be used with different concentration and volume units as long as they are the same on both sides.)

> The formula $c_1V_1 = c_2V_2$ can be used when solving problems involving the dilution of solutions. Units of c and V must be the same on both sides of the formula.

Worked example 13.5.6

QUESTIONS INVOLVING DILUTION

Calculate the concentration of the solution formed when 10.0 mL of water is added to 5.00 mL of 1.2 M HCl.	
Thinking	**Working**
Write down the value of c_1 and V_1. Note: c_1 and V_1 refer to the original solution, before water was added.	$c_1 = 1.2\,M$ $V_1 = 5.00\,mL$
Write down the value of V_2. Note: V_2 is the total volume of the original solution plus the added water.	$V_2 = 10.0 + 5.00$ $= 15.0\,mL$
Transpose the equation $c_1V_1 = c_2V_2$ to allow calculation of the concentration, c_2, of the new solution.	$c_1V_1 = c_2V_2$ $c_2 = \frac{c_1V_1}{V_2}$
Calculate the concentration of the diluted solution.	$c_2 = \frac{1.2 \times 5.00}{15.0}$ $= 0.40\,M$

➤ Try yourself 13.5.6

QUESTIONS INVOLVING DILUTION

Calculate the concentration of the solution formed when 95.0 mL of water is added to 5.00 mL of 0.500 M HCl.

Changing the units of concentration

At times it is useful to change, or 'convert', concentration values from one unit to another unit. One way to do this is in a series of simple steps. Worked example 13.5.7 shows how this can be done.

Worked example 13.5.7

CONCENTRATION UNIT CONVERSIONS

Determine the concentration, in ppm, of a 0.00200 M solution of NaCl. Remember that concentration in ppm is the same as $mg\,L^{-1}$.	
Thinking	**Working**
Calculate the number of moles of solute in 1.00 L of the solution.	$n(NaCl) = c \times V$ $= 0.00200 \times 1.00$ $= 0.00200\,mol$
Calculate the mass, in grams, of solute in 1.00 L of the solution.	$M(NaCl) = 35.45 + 22.99$ $= 58.44\,g\,mol^{-1}$ $m(NaCl) = n \times M$ $= 0.00200 \times 58.44$ $= 0.117\,g$
Calculate the mass, in mg, of solute in 1.00 L of the solution.	$m(NaCl) = 0.117 \times 1000$ $= 117\,mg$
Express the concentration of the solute in ppm.	$c(NaCl) = 117\,ppm$

➤ Try yourself 13.5.7

CONCENTRATION UNIT CONVERSIONS

Calculate the concentration, in ppm, of a 0.0100 M solution of NaOH. Remember that concentration in ppm is the same as $mg\,L^{-1}$.

13.5 Review

SUMMARY

- The concentration of a solution is defined as the quantity of solute dissolved in a quantity of solution.
- Concentration units have two parts. The first part provides information about the quantity of solute. The second part provides information about the quantity of solution.
- The concentrations of solutions can be expressed in different units including $g\,L^{-1}$, $mg\,L^{-1}$, %(m/m), %(m/v), %(v/v) and ppm.
- Molarity is defined as the number of moles of solute per litre of solution.
- Molarity is calculated using the formula $c = \frac{n}{V}$, where c is the concentration in $mol\,L^{-1}$, n is the number of moles and V is the volume in litres.
- The formula $n = c \times V$ can be used to calculate the number of moles of solute in a given volume of solution.
- Numerical problems involving dilution can be solved using the formula:
  $c_1V_1 = c_2V_2$
  where c is the concentration and V is the volume. When using this formula, c_1 and c_2 must be in the same units of concentration and V_1 and V_2 must be in the same units of volume.
- One type of concentration unit can be converted to another unit in simple steps. For example, units of %(m/m) can be converted to units of $mol\,L^{-1}$.

KEY QUESTIONS

Describe

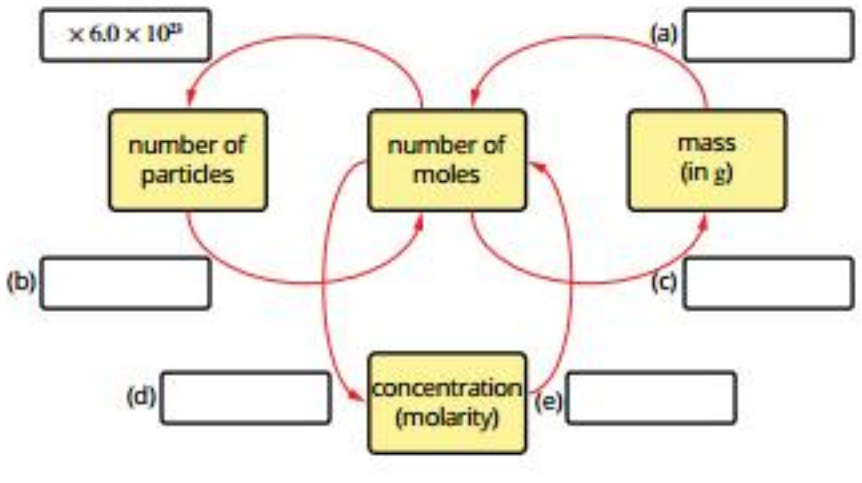
1 A laboratory contains a large bottle of hydrochloric acid labelled 6.5 M. What is the significance of the 6.5 M on the label?

2 An aqueous solution is diluted with more water. For each of the following characteristics, state whether during dilution each characteristic increases, decreases or does not change.
- **a** mass of solution
- **b** concentration of solution
- **c** mass of solute
- **d** volume of solution
- **e** number of moles of solute

3 Describe what measures of concentration are used for household products like cleaning agents and alcohol.

Apply

4 Fill in the blanks in the figure below, in order to construct a flow chart for performing these calculations.



5 A 50 g sample of sucrose is dissolved in water. Identify the solute, the solvent and the solution.

6 Explain why ppm is a more commonly used measure for the concentration of mercury in fish for human consumption rather than $mol\,L^{-1}$ or %(m/m).

Analyse

7 Calculate the molar concentrations of the following solutions.
- **a** 50.0 mL solution that contains 0.17 mol of KNO_3
- **b** 2.4×10^3 L solution that contains 85 mol of NaCl
- **c** 1.25 L solution that contains 4.6 g of NH_4Br

8 Calculate the amount, in mol, of solute in each of the following solutions.
- **a** 0.50 L of a 0.40 M $CaCl_2$ solution
- **b** 22.4 mL of a 0.025 M KCl solution

9 Calculate the mass, in grams, of solute in each of the following solutions.
- **a** 1.3 L of a 0.025 M $FeCl_3$ solution
- **b** 25.0 mL of a 1.75 M NH_4Cl solution

10 Calculate the concentration of the following solutions in ppm.
- **a** 25 mg sample of $CaCl_2$ dissolved in 5.0 kg of solution
- **b** 1.25 g sample of lead nitrate dissolved in 2000 g of solution

11 Calculate which of the following is the most concentrated solution: 5.00 g of NaCl in 100 mL of water or 2.00 M NaCl.

12 Calculate the concentration of a 200 mL solution that contains 4.56 g of barium sulfate.

13.5 Review *continued*

13 Calculate the final concentration of each of the following diluted solutions.

a 10.0 mL sample of water added to 5.0 mL of 1.2 M HCl

b 1.0 L sample of water added to 3.0 L of 0.10 M HCl

14 What volume, in mL, of a 0.20 M NaCl solution would be required to prepare 80.0 mL of a 0.050 M solution of the compound?

15 When 5.6 mL of a 0.16 M solution of KNO_3 was diluted, the concentration of the diluted solution was 0.024 M. What was the volume of water, in mL, that was added to the original solution?

16 The concentration of a solution of NaOH is 17.0%(m/v). Calculate the concentration of this solution in mol L^{-1}.

17 The concentration of a solution of ammonia (NH_3) is 1.5%(m/v). Determine the molar concentration of a solution produced by diluting 25.0 mL of this solution with 250 mL of water.

18 Referring to Figure 13.5.3 on page 379, determine the concentration of alcohol in mol L^{-1}. (Assume the alcohol is ethanol C_2H_5OH; density of ethanol is 0.7893 g cm^{-3}.)

Chapter review

13

KEY TERMS

aqueous
concentrated solution
crystallise
density
dilute solution
dilution
dipole
dissociation
dissolution
electronegativity
electrostatic attraction
force
full equation
homogeneous
hydrated
hydride
hydrogen bond
hydrogen bonding
hydronium ion
immiscible
intermolecular force
intramolecular bond
ion–dipole attraction
ionic equation
ionise
latent heat
latent heat of fusion
latent heat of vaporisation
lone pair
miscible
molar concentration
molarity
non-polar
parts per million (ppm)
polar
precipitate
precipitation reaction
saturated solution
seed crystal
solubility
solubility curve
solubility table
solute
solution
solvent
specific heat capacity
spectator ion
supersaturated solution
surface tension
unsaturated solution

KEY QUESTIONS

Describe

1 Hydrogen peroxide solutions for hair bleaching are sold as 120 mL solutions containing 5.00 g of H_2O_2 dissolved in water. Determine the molar concentration of hydrogen peroxide in the bleaching product.
A 0.81 %(m/v)
B 1.23 M
C 41.7 gL^{-1}
D 1.23×10^{-3} $molmL^{-1}$

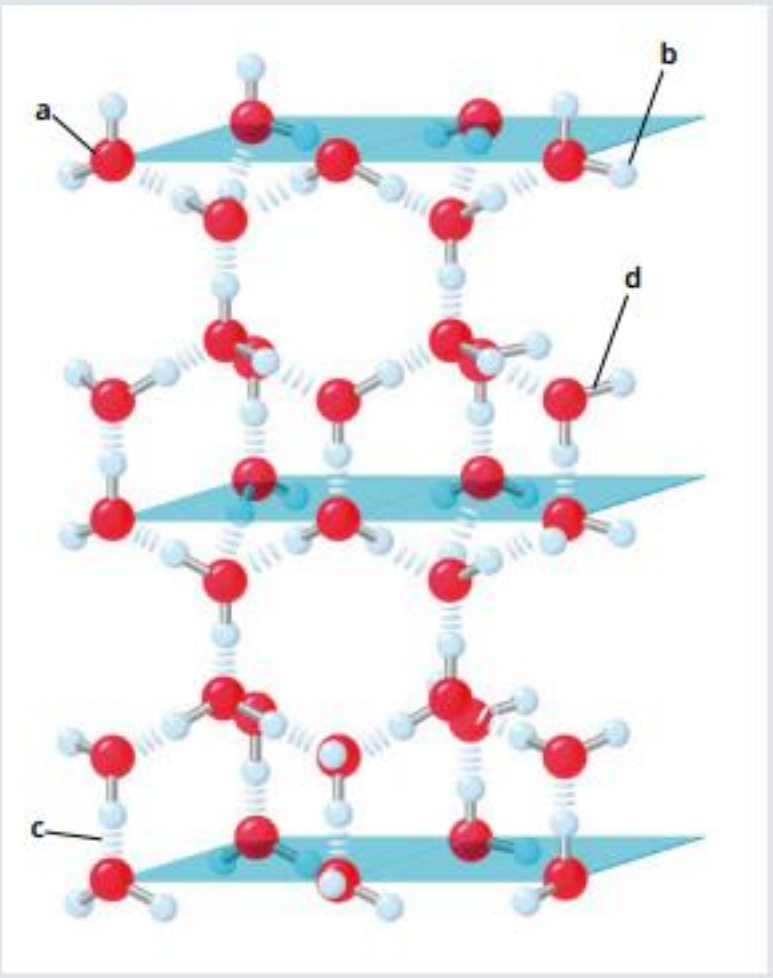
2 Identify which of the following intermolecular forces gives water its unique physical properties.
A dispersion forces
B covalent bonds
C hydrogen bonds
D dipole–dipole interactions

3 Determine which one of the following ionic compounds would be insoluble in water.
A sodium nitrate
B ammonium chloride
C barium sulfate
D iron (II) chloride

4 Identify which one of the following substances would dissolve in water by forming hydrogen bonds.
A ammonia (NH_3)
B hexane (C_6H_{14})
C sodium chloride (NaCl)
D hydrogen chloride (HCl)

5 The spectator ions present when a solution of barium nitrate is added to a solution of sodium sulfate are:
A Ba^{2+} and Na^+ ions
B NO_3^- and Ba^{2+} ions
C SO_4^{2-} and Na^+ ions
D Na^+ and NO_3^- ions

6 The image below shows the arrangement of water molecules in ice. Identify the parts of the diagram labelled **a–d**.



7 Many of the solvent properties of water depend on its structure and bonding. List all the bonds present in a sample of water from weakest to strongest. Remember to include all intramolecular and intermolecular bonding.

8 Describe what happens to the forces between solute and solvent substances when an ionic substance such as potassium bromide dissolves in water.

9 Explain why water is such a good solvent for polar and ionic substances.

10 Methanol (CH_3OH) and ethanoic acid (CH_3COOH) dissolve in water. Write chemical equations to represent the dissolving process for each of these compounds.

11 Write the equations to show the dissociation of the following compounds when they are added to water.
- **a** magnesium sulfate
- **b** sodium sulfate
- **c** potassium hydroxide
- **d** copper(II) ethanoate

12 Calculate the molar concentration of a 1.55 L solution that contains 1.223 g of $CaCl_2$.

13 Match the following terms with their definitions:
latent heat of fusion, specific heat capacity, latent heat of vaporisation, boiling point
- **a** the temperature at which a liquid boils to form a gas
- **b** the heat energy required to melt a solid to a liquid at its melting point
- **c** the amount of heat energy required to increase 1 g of a substance by 1°C
- **d** the heat energy required to evaporate a liquid to a gas at its boiling point

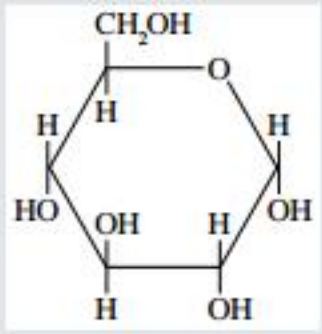
Apply

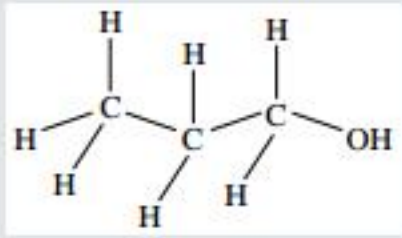
14 Consider the following ions: SO_4^{2-}, PO_4^{3-}, Br^-, S^{2-}. Determine which of these would combine with $Fe^{3+}(aq)$ to form a precipitate.

15 What precipitate will be formed (if any) when the following solutions are mixed?
- **a** barium nitrate and sodium sulfate
- **b** sodium chloride and copper(II) sulfate
- **c** magnesium sulfate and lead(II) nitrate
- **d** potassium chloride and barium nitrate

16 Hydrogen sulfide and water are both group 16 hydrides. Explain why water exhibits a much higher boiling point than hydrogen sulfide and the other group 16 hydrides.

17 Classify the following substances according to the way they dissolve in water: $C_6H_{12}O_6$, HI, I_2, C_2H_4, C_3H_7OH, HNO_3, CH_4.
The structures of $C_6H_{12}O_6$ and C_3H_7OH are shown below to assist you.





18 Explain, with reference to its structure and bonding, why octane does not dissolve in water.

19 Sugar is soluble in water. Explain the three steps involved when sugar molecules dissolve to form an aqueous sugar solution.

20 Water is added to 50.0 mL of 5.00 M HCl until the total volume is 250 mL. Calculate the concentration of HCl in the diluted solution.

21 A 1.50 mL sample of a 0.0500 M solution of calcium chloride ($CaCl_2$) was diluted with water to a volume of 10.0 L. Determine the concentration of Cl^- ions in the diluted solution in ppm.

22 In your own words, discuss the significance of polarity and hydrogen bonding in relation to the high boiling point of water.

Analyse

23 Write full balanced chemical equations and ionic equations for each of the following precipitation reactions.
- **a** $NH_4Cl(aq) + AgNO_3(aq)$
- **b** $FeCl_2(aq) + Na_2S(aq)$
- **c** $Fe(NO_3)_3(aq) + KOH(aq)$
- **d** $CuSO_4(aq) + NaOH(aq)$
- **e** $Ba(NO_3)_2(aq) + Na_2SO_4(aq)$

24 Calculate the concentration, in $g\,L^{-1}$, of a 60 mL solution that contains 5.0 g of sugar.
- **A** 300
- **B** 53
- **C** 12
- **D** 83

25 Nitrogen gas (N_2) and ethene (C_2H_6) are both insoluble in water, whereas ethanol (C_2H_5OH) is soluble. Refer to the bonding in each of the molecules to explain these differences.

26 DDT is a hazardous agricultural insecticide, which has been banned in many countries. It is only slightly soluble in water but is very soluble in fats and oils, so accumulates in the fat deposits of animals. Use the skills you have gained from this chapter to deduce the polarity of the DDT molecule from its solubility characteristics.

27 Use Figure 13.3.2 on page 362 to deduce the minimum temperature required to dissolve 40 g of $AgNO_3$ in 25 g of water.

28 Refer to Figure 13.3.2 on page 362 to answer the following.
A saturated solution of sodium nitrate was prepared by dissolving the maximum amount of solute in water at 50°C.
What mass will dissolve in 150 g of water.

29 Explain what happens to the forces between solute and solvent substances when an ionic substance such as potassium bromide dissolves in water.

30 Determine the molar concentration of a saturated $CuSO_4.5H_2O$ solution at 20°C. (Assume that 1 g of water gives 1 mL of solution.)

31 Compare and contrast the dissolution of ionic substances and molecular substances that ionise in water.

32 Identify the ions produced when the following compounds are added to water.
- **a** $Cu(NO_3)_2$
- **b** $ZnSO_4$
- **c** $(NH_4)_3PO_4$

33 Water boils at 100°C. However, a much higher temperature (1000°C) is needed to decompose water molecules into hydrogen gas and oxygen gas.
- **a** Using water as an example, explain the meaning of the terms 'intermolecular' and 'intramolecular' forces.
- **b** Determine which of the two types of force in part **a** is stronger. Justify your answer by using the information at the beginning of the question.

34 Calculate the molar concentration of a sodium sulfate solution that has a concentration of 4.26%(m/v).

35 Identify three sulfate compounds that have these characteristics.
- **a** soluble in water
- **b** insoluble in water

36 Calculate the volume of 10 M HCl needed to prepare 200 mL of 0.45 M HCl solution.

37 Categorise the following as soluble or insoluble.
- **a** copper(II) chloride
- **b** silver iodide
- **c** barium hydroxide
- **d** lead(II) sulfate
- **e** potassium nitrate

38 In each 5.0 mL dose of a cold and flu medicine, there is 2.00 mg of the active ingredient. Calculate the concentration of this chemical in:
- **a** $mg\,L^{-1}$
- **b** %(m/v)

39 Calculate the final volume of a solution of NaOH if 200 mL of a 0.500 M solution was diluted to 0.200 M.

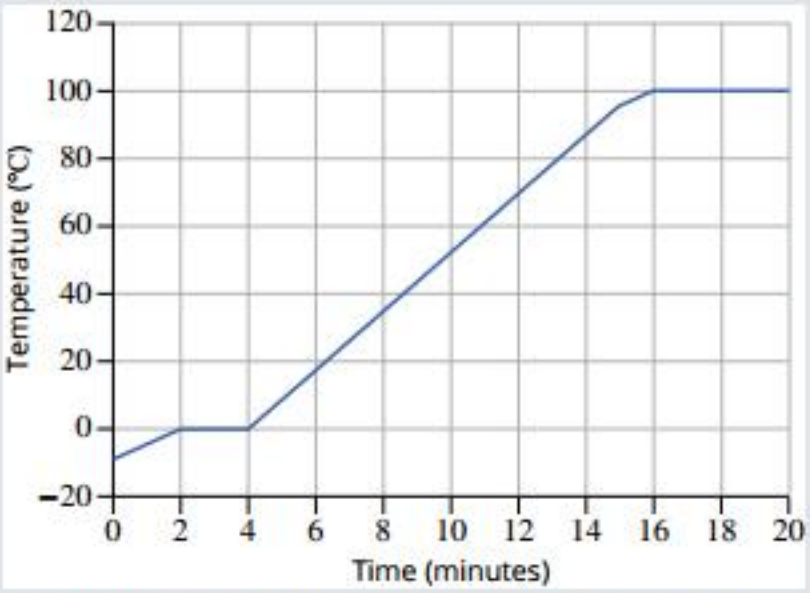
40 Calculate the concentration of a 0.00400 M solution of potassium nitrate (KNO_3) in ppm.

41 Use Table 13.3.2 on page 366 to help you answer this question.
- **a** Using data from the table, make a general statement about the relationship between the amount of gas dissolved in water as the temperature increases.
- **b** When a saucepan of cold water is heated on a stove, bubbles of gas appear on the bottom of the saucepan long before the water boils. Explain this observation.
- **c** A litre of water weighs 1 kg. A bucket of water at 20°C contains 0.24 g of dissolved oxygen. What is the volume of water in the bucket?

Interpret

42 An evaporative air conditioner is used to cool the air inside some buildings. The cooler lowers the air temperature by using heat from the air to evaporate water. Which property is most important when water is used in an evaporative air conditioner?

43 A student was asked to record the temperature changes as a sample of ice was heated. The ice was placed in a beaker and heated with a Bunsen burner for 20 minutes. The graph below shows the temperature, in degrees Celsius, recorded at 1 minute intervals.



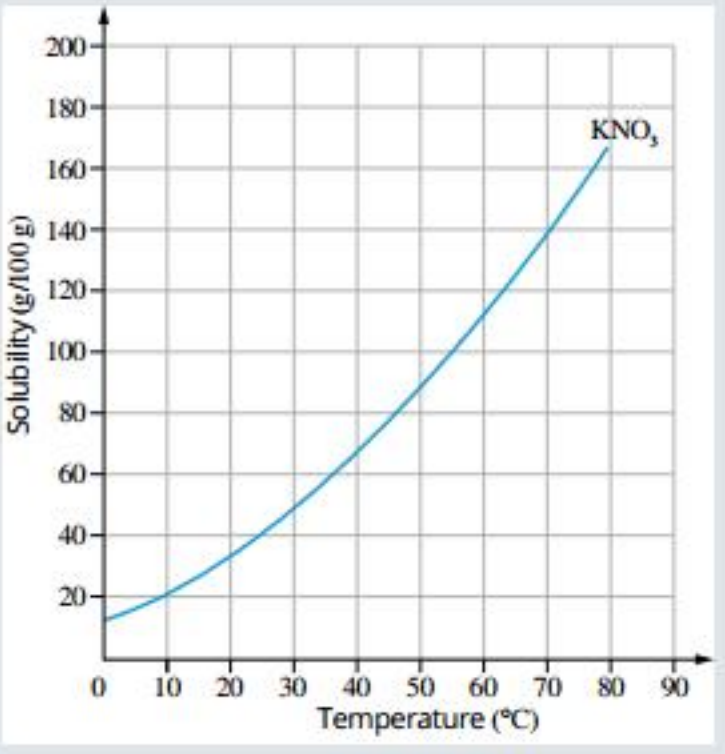
- **a** Explain what is happening, at a molecular level, between 2 and 4 minutes on the graph.
- **b** Even though heating is continued for 20 minutes, no further temperature rise is observed after 16 minutes. Explain what happens to the added heat between 16 and 20 minutes.

44 A student conducts an experiment to investigate the solubility of CH_4 and CH_3OH molecules in three different solvents, X, Y and Z. The student finds that the CH_3OH molecules dissolve well in solvent Y but do not dissolve in solvent X. The student also finds that CH_4 partially dissolves in solvent Z and completely dissolves in solvent X. List each of the solvents in order from most polar to least polar. Explain your reasoning.

45 Glucose ($C_6H_{12}O_6$) and common salt (NaCl) both form clear colourless solutions when dissolved in water. Suggest an experiment you could perform in the laboratory to tell the two solutions apart.

46 The following question refers to the solubility curve of potassium nitrate (KNO_3) shown in the figure below.

- **a** Determine the mass of potassium nitrate that will dissolve in 500 g of water at 70°C.
- **b** If 50 g of water at 70°C contained 25 g of KNO_3, determine how much more KNO_3 must be added to make a saturated solution.
- **c** If 100 g of KNO_3 is added to 50 g of water at 40°C, calculate the mass of KNO_3 that will not dissolve.
- **d** Calculate the molar concentration of the potassium nitrate solution prepared in part **c**. (Assume that 1 g of water gives 1 mL of solution.)



Data analysis

DATA SET 1

The information below applies to Questions 1–5.

An important part of chemistry is qualitative analysis—the process of finding out what substances are present in an unknown sample. Precipitate formation can be used to identify unknown cations and anions, thereby providing clues about the substances present in a sample. A student was provided with a set of solutions identified only by the letters A–F. Each one of the unknown solutions corresponds to one of the following substances:

water

0.1 M sulfuric acid, $H_2SO_4(aq)$

0.1 M zinc chloride, $ZnCl_2(aq)$

0.1 M sodium chloride, NaCl(aq)

0.1 M sodium hydroxide, NaOH

0.1 M sodium carbonate, $Na_2CO_3(aq)$

The student performed a number of tests on the unknown solutions. The experimental data collected by the student is shown in Table 1.

TABLE 1 Logbook data for ion identification

Unknown solution	Observations when tested with	
	silver nitrate(aq)	**barium nitrate(aq)**
A	brown	cloudy
B	white	no observable reaction
C	white	no observable reaction
D	no observable reaction	white
E	light brown	white
F	no observable reaction	no observable reaction

Table 2 gives a brief description of precipitates formed when various cations and anions react.

TABLE 2 Formation of precipitates

Cations used to identify the anion	Anions used to identify the cation							
	nitrate NO_3^-	**sulfate SO_4^{2-}**	**carbonate CO_3^{2-}**	**chloride Cl^-**	**iodide I^-**	**bromide Br^-**	**hydroxide OH^-**	**hydroxide (OH^-) with ammonia (NH_3) added**
sodium Na^+								
potassium K^+								
barium Ba^{2+}		white	white				cloudy	
calcium Ca^{2+}			cloudy white				cloudy	
aluminium Al^{3+}			cloudy				cloudy (light)	cloudy
zinc Zn^{2+}			cloudy				cloudy	
iron(II) Fe^{2+}			grey-green				green	light green
iron(III) Fe^{3+}							brown	brown
copper Cu^{2+}			light blue		mustard		blue	
lead Pb^{2+}		white	white	cloudy	yellow	cloudy	white	white
silver Ag^+			light brown	white	light yellow	cream	brown	

Formation of precipitates:
White, green, yellow and so on means the precipitate is visible on the bottom of the test tube.
Cloudy means the precipitate is uniformly suspended in the water.
For blank spaces, the substance is assumed to be soluble, giving a clear (possibly coloured) solution.

The laboratory technician prepared the solutions for the students. A 3.5 M sulfuric acid solution was diluted to prepare 150 mL of the 0.10 M sulfuric acid (H_2SO_4) solution. The 0.10 M sodium chloride (NaCl) solution was prepared by dissolving an accurately measured mass of sodium chloride and dissolving the solid in water to a volume of 150 mL.

Question 1 (2 marks)

Calculate the mass of sodium chloride required to prepare 150 mL of 0.10 M NaCl solution for the students.

Question 2 (1 mark)

Calculate the volume of 3.5 M sulfuric acid solution required to prepare 150 mL of 0.10 M H_2SO_4 solution for the students.

Question 3 (1 mark)

The students were able to identify four of the unknown solutions using the data in Table 1. Which two solutions (A–F) cannot be identified based on the data?

Question 4 (2 marks)

Suggest one additional precipitation test that could be performed to identify the two solutions in Question **3**. Include the expected observations in your answer.

Question 5 (4 marks)

Use the experimental data in Table 1 to identify the other four unknown solutions.

CHAPTER

14 An introduction to acids and bases

Acids and bases are among the most important types of electrolytes. They play a key role in many environmental, industrial and biochemical applications and they make up some of the household products in your kitchen and laundry. In this chapter, you will be introduced to the Arrhenius model to help explain the chemical properties of acids and bases. You will also look at how electrolytes such as acids and bases can be characterised as either strong or weak, and you will be introduced to how the acidity (or basicity) of a solution can be quantified using the pH scale. Lastly, the reactions of acids and bases will be investigated, enabling you to predict the products of a variety of reactions involving acids and bases.

Syllabus subject matter

Topic 2 • Aqueous solutions and acidity

■ AQUEOUS SOLUTIONS AND MOLARITY

- Discriminate between the terms *strength* and *concentration*, e.g. acidic/basic solutions. **14.1**
- State that square brackets ([ ]) are used to denote concentration. **14.2**

■ pH

- State that pH is dependent on the concentration of hydrogen ions in solution. **14.2**
- Identify that the pH scale is a logarithmic scale. **14.2**
- Apply the pH scale to compare the levels of acidity or alkalinity of aqueous solutions. **14.2**
- Apply the Arrhenius model to explain the behaviour of strong and weak acids and bases in aqueous solutions. **14.1**

■ REACTIONS OF ACIDS

- Determine balanced chemical and ionic equations (including states) for the reactions of acids with bases, metals and carbonates. **14.3**

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14.1 Introducing acids and bases

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- explain the properties of acids and bases using the Arrhenius model
- discriminate between strong and weak acids and bases.

Acids are used in your home, in agriculture and in industry (Figure 14.1.1). They also have an important role in your body. In this module, you will be introduced to the Arrhenius model that explains the chemical properties of acids and bases, helping you to explain their usefulness within the home and industry. You will also look at how the **acidity** of a solution can be determined, and how acids and bases can be characterised as either strong or weak.

FIGURE 14.1.1 Common household products that contain acids, bases or salts.

Table 14.1.1 gives the names, chemical formulas and uses of some common acids.

TABLE 14.1.1 Common acids and their everyday uses

Name	Formula	Uses
hydrochloric acid	HCl	present in stomach acid to help break down proteins as a cleaning agent for brickwork
sulfuric acid	H_2SO_4	one of the most common chemicals manufactured in car batteries and in the manufacture of fertilisers and detergents
nitric acid	HNO_3	in the manufacture of fertilisers, dyes and explosives
ethanoic acid (acetic acid)	CH_3COOH	found in vinegar as a preservative
carbonic acid	H_2CO_3	found in carbonated soft drinks and beer
phosphoric acid	H_3PO_4	in some soft drinks and in the manufacture of fertilisers
citric acid	$C_6H_8O_7$	found in citrus fruits
ascorbic acid	$C_6H_8O_6$	found in citrus fruits (vitamin C)

Many cleaning agents used in the home, such as washing powders and oven cleaners, contain **bases**. **Solutions** of ammonia are used as floor cleaners, and sodium hydroxide is the major active ingredient in oven cleaner. Bases are effective cleaners because they react with fats or oils to produce water-soluble soaps. A soluble base is referred to as an **alkali**. Not all bases are soluble. Calcium carbonate will react with acids but is insoluble in water so is not considered an alkali.

Table 14.1.2 gives the names, chemical formulas and uses of some common bases.

Aqueous solutions of bases are called alkalis.

TABLE 14.1.2 Common bases and their everyday uses

Name	Formula	Uses
sodium hydroxide (caustic soda)	$NaOH$	drain and oven cleaners, and soap making
ammonia	NH_3	household cleaners, fertilisers and explosives
calcium hydroxide	$Ca(OH)_2$	found in cement and mortar in garden lime to adjust soil pH
magnesium hydroxide	$Mg(OH)_2$	key ingredient in some antacids, such as milk of magnesia, to overcome indigestion
sodium carbonate	Na_2CO_3	in the manufacture of washing powder and glass

All acids have some properties in common. Bases also have common properties. The properties of acids and bases are summarised in Table 14.1.3.

TABLE 14.1.3 Properties of acids and bases

Properties of acids	Properties of bases
turn litmus indicator red	turn litmus indicator blue
tend to be corrosive	are caustic and feel slippery
taste sour	taste bitter
react with bases	react with acids
solutions have a relatively low pH	solutions have a relatively high pH
solutions conduct an electric current	solutions conduct an electric current

CHANGING IDEAS ABOUT THE NATURE OF ACIDS AND BASES

Over the years, there have been many attempts to define acids and bases. At first, acids and bases were defined in terms of their observed properties such as their taste, effect on **indicators** and reactions with other substances.

For example, in the seventeenth century, British scientist Robert Boyle described the properties of acids in terms of taste, their action as solvents and how they changed the colour of certain vegetable extracts (similar to red cabbage juice seen in Figure 14.1.2). He also noticed that alkalis (soluble bases) could reverse the effect that acids had on these extracts.

It was not until the late eighteenth century that attempts were made to define acids and bases on the basis of the nature of their constituent elements. Antoine Lavoisier, a French chemist, thought that acidic properties were due to the presence of oxygen. While this explanation applied to sulfuric acid (H_2SO_4), nitric acid (HNO_3) and phosphoric acid (H_3PO_4), it did not explain why hydrochloric acid (HCl) was an acid.

In about 1810, Humphry Davy suggested that the acidic properties of substances were associated with hydrogen and not oxygen. He came to this conclusion after producing hydrogen gas by reacting acids with metals. Davy also suggested that acids react with bases to form salts and water.

FIGURE 14.1.2 Natural acid–base indicators are found in plants such as red cabbage. Red cabbage extract turns a different colour in (from left to right) strong acid, weak acid, neutral solution, weak base and strong base.

This theory was further developed by the Swedish scientist Svante Arrhenius. In 1887, he defined acids and bases as follows.

- Acids are substances that **dissociate** (break apart) and **ionise** (form ions) in water. They produce hydrogen ions (H^+).
- Bases are substances that dissociate in water to produce **hydroxide ions** (OH^-).

THE ARRHENIUS MODEL OF ACIDS

In the Arrhenius model, an acid is defined as a substance that ionises in water to produce hydrogen ions (H^+). For example, when hydrogen chloride gas (HCl(g)) is bubbled through water, the HCl molecules break apart and ionise to form hydrochloric acid (HCl(aq)), which consists of hydrogen ions and chloride ions in the aqueous solution:

$$HCl(g) \xrightarrow{H_2O} HCl(aq) \rightarrow H^+(aq) + Cl^-(aq)$$

Arrhenius acids in their pure form do not contain ions; the ions are formed via a chemical reaction with water:

$$HCl(g) + H_2O(l) \rightarrow H_3O^+(aq) + Cl^-(aq)$$

You will recall from the previous chapter that as soon as H^+ ions are formed in water they immediately react with water molecules to produce the **hydronium ion** (H_3O^+). For this reason, you may also recall that the notation for hydrogen ions (H^+) and hydronium ions (H_3O^+) are sometimes used interchangeably.

The Arrhenius model of acids is useful because it explains the similarities in the reactions of different acids. The hydrogen ions that are present in acid solutions account for the common properties of acids, including their reactions with bases, carbonates and metals. For example, as you will see later in this chapter, the hydrogen ions present in all acid solutions form hydrogen gas when the acid reacts with metals such as magnesium:

$$2H^+(aq) + Mg(s) \rightarrow H_2(g) + Mg^{2+}(aq)$$

THE ARRHENIUS MODEL OF BASES

Arrhenius defined a base as a substance that dissociates in water to form hydroxide ions. Sodium hydroxide is a soluble ionic compound, containing sodium ions and hydroxide ions. When it is added to water it dissociates:

$$NaOH(s) \rightarrow Na^+(aq) + OH^-(aq)$$

Some bases dissociate to form more than one hydroxide ion:

$$Ca(OH)_2(s) \rightarrow Ca^{2+}(aq) + 2OH^-(aq)$$

The presence of the hydroxide ions in solutions of bases accounts for the common properties of Arrhenius bases. For example, the hydroxide ion reacts with the litmus indicator to form a blue-coloured compound.

LIMITATIONS OF THE ARRHENIUS THEORY OF ACIDS AND BASES

The Arrhenius model explains the properties of acids and bases in terms of the formation of hydrogen ions by **ionisation** of the acid molecule or hydroxide ions by **dissociation** of the base molecule. However, the model does have some limitations.

The model does not explain why some substances that do not contain hydrogen form acidic solutions when mixed with water. For example, acidic solutions are formed when carbon dioxide, CO_2, or sulfur dioxide, SO_2, are dissolved in water. The model also does not explain why some substances such as ammonia, NH_3, or sodium hydrogen carbonate, $NaHCO_3$, form basic solutions when mixed with water, even though they do not contain hydroxide ions.

The Arrhenius model is also restricted to acids and bases that dissolve in water. The model does not explain acid–base behaviour in non-aqueous solutions.

HCl can refer to two different substances. At room temperature and pressure, the molecular compound hydrogen chloride exists as a gas, HCl(g). Only when dissolved in water is it called hydrochloric acid, HCl(aq). Since HCl fully ionises in water, HCl(aq) can also be represented as separate $H^+(aq)$ ions and $Cl^-(aq)$ ions.

Dissociation is a process where a compound breaks apart into its constituent parts (normally ions), for example, when ionic NaOH(s) forms Na^+ and OH^- ions upon dissolving in water.

Ionisation is a process where ions are formed from a substance that does not initially contain ions, for example, the formation of H^+ and Cl^- ions from molecular hydrogen chloride (HCl).

An Arrhenius acid is defined as a substance that dissociates and ionises in water to produce hydrogen ions (H^+). They are molecular compounds.

An Arrhenius base is defined as a substance that dissociates in water to produce hydroxide ions (OH^-). They are generally ionic compounds.

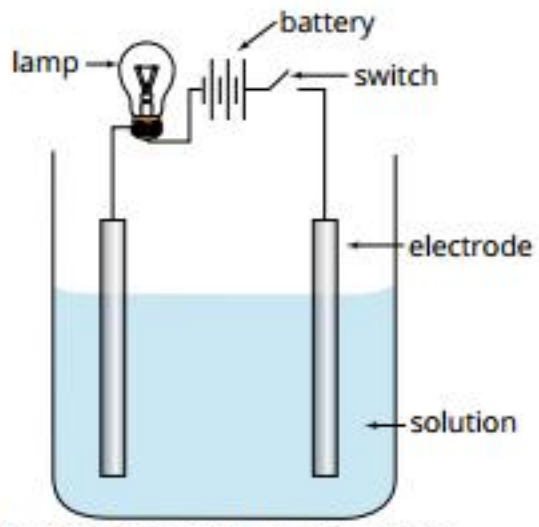
An improved model for acid–base behaviour is the Brønsted–Lowry model, which describes an acid as a substance that can donate a hydrogen ion to a base, which accepts it. Recall that a hydrogen ion is a proton—the nucleus of a hydrogen atom that has been separated from its accompanying electron. You will learn more about the Brønsted–Lowry model in Unit 3.

ACIDS AND BASES AS ELECTROLYTES

According to the Arrhenius model, acids dissociate and ionise in water to produce hydrogen ions (H^+), whereas bases dissociate in water to produce hydroxide ions (OH^-). The production of these charged particles in solution allows acids and bases to conduct electricity.

Dissolved ions become highly mobile in an electric field and can maintain an electrical current in an aqueous solution, as shown in Figure 14.1.3. Relatively high electrical conductivity corresponds to relatively high concentrations of ions in solution; relatively low electrical conductivity corresponds to relatively low concentrations of ions in solution.

For example, hydrochloric acid is formed when hydrogen chloride ionises in water to form a solution containing hydrogen ions and chloride ions. When a solution of hydrochloric acid is tested with the conductivity apparatus shown in Figure 14.1.3, the lamp (light globe) will glow. The chloride ions are attracted to the positive electrode of the apparatus and the hydrogen ions to the negative electrode. The movement of these ions creates a flow of current in the solution that makes the lamp glow.



If the solution conducts an electric current, the lamp glows.

FIGURE 14.1.3 Apparatus used to test the conductivity of acid solutions.

Electrolytes and non-electrolytes

Substances that dissolve in water to produce electrically conducting solutions are called **electrolytes**. All ionic compounds that are soluble in water are electrolytes. By contrast, ionic compounds that do not dissolve in water (and therefore do not release ions into solution) are not electrolytes.

For example, common table salt, sodium chloride (NaCl), is an ionic compound made up of positively charged sodium **cations** (Na^+) and negatively charged chloride **anions** (Cl^-). When NaCl is dissolved in water, the crystal lattice breaks apart and individual Na^+ and Cl^- ions are released into solution. This dissolution process can be represented as follows:

$$NaCl(s) \xrightarrow{H_2O} NaCl(aq) \rightarrow Na^+(aq) + Cl^-(aq)$$

where NaCl(aq) refers to dissolved sodium chloride, which can also be represented as individual ions in solution.

Not all substances that dissolve in water are electrolytes. Common table sugar, or sucrose, is an example of a non-electrolyte, which means that it is a substance that dissolves in water to produce an electrically non-conducting (or poorly conducting) solution. Sucrose is a molecular compound with the formula $C_{12}H_{22}O_{11}$. Recall that **molecules** are not made up of ions; they are chemically bonded groups of non-metallic atoms held together by covalent bonds. When sucrose dissolves in water, its molecular structure stays intact and no ions are produced. We can represent this dissolution process as follows:

$$C_{12}H_{22}O_{11}(s) \xrightarrow{H_2O} C_{12}H_{22}O_{11}(aq)$$

All ionic compounds that are soluble in water are electrolytes, but not all electrolytes are formed from ionic compounds. For example, some molecular compounds such as hydrogen chloride (HCl) ionise in water to produce freely mobile ions and an electrically conducting solution. Acids such as HCl are the most important class of molecular compounds that are electrolytes.

Strong and weak electrolytes

Electrolytes can be classified as either strong electrolytes or weak electrolytes. A **strong electrolyte** is a substance that, when dissolved in water, completely ionises or dissociates into ions. A **weak electrolyte** is a substance that, when dissolved in water, only slightly ionises or dissociates into ions. The ionic compounds NaCl, NaOH and $Ca(OH)_2$ are all examples of strong electrolytes.

To determine which ionic compounds are strong electrolytes, we can refer to the solubility rules from the previous chapter. For example, all Group 1 metal salts, all nitrate salts, all ethanoate salts and all ammonium salts are highly soluble in water. Their high solubility is the result of almost complete dissociation of their ions when dissolved and, therefore, all of these compounds would be considered strong electrolytes. Ionic salts that are sparingly soluble (or partially soluble) at a particular temperature would be considered weak electrolytes. Salts considered to be insoluble would not be classified as electrolytes, or they may be considered very weak electrolytes if they dissociate only to a very limited extent.

For molecular compounds, the situation is more complex with some completely ionising when dissolved in water (e.g. HCl), some not ionising at all (e.g. sucrose) and some ionising to only a limited extent. The most common examples of weak electrolytes are organic acids such as citric acid (found in citrus fruits), ethanoic acid (found in vinegar) and ascorbic acid (vitamin C). Some inorganic acids such as nitrous acid ($HNO_2(aq)$) and hydrofluoric acid (HF(aq)) are also weak electrolytes. The partial ionisation of HF can be represented as follows:

$$HF(g) \xrightleftharpoons{H_2O} H^+(aq) + F^-(aq)$$

or

$$HF(g) + H_2O(l) \rightleftharpoons H_3O^+(aq) + F^-(aq)$$

The double arrows in these chemical equations mean that these chemical processes are significant in both directions. At the same time as the HF molecules are undergoing ionisation (the forward direction), the ions are re-combining (or re-configuring) to produce the HF molecule (the reverse direction). The balance between the forward and reverse reactions is known as a chemical equilibrium. Chemical equilibrium processes are covered in Unit 3.

Organic bases such as pyridine and urea are other examples of weak electrolytes.

Strong and weak acids and bases

Acids and bases that are strong electrolytes are known as **strong acids** and **strong bases**. Conversely, acids and bases that are weak electrolytes are known as weak acids and weak bases.

According to the Arrhenius model, the stronger an acid is, the more easily it ionises and dissociates in water to produce hydrogen ions. These ions immediately react with the water molecules to form the hydronium ion (H_3O^+). The stronger an Arrhenius base is, the more easily it dissociates to form the hydroxide (OH^-) ion. Strong acids and bases dissociate readily and therefore conduct electricity to a greater degree than weak acids and bases that do not dissociate in water to the same extent.

Hydrochloric acid is considered a strong acid because hydrogen chloride (HCl) dissolves (or ionises) almost completely in water and exists almost exclusively as H^+ ions and Cl^- ions in solution. For our study purposes, there are only seven acids that become fully ionised when dissolved in water. These seven strong acids are listed in Table 14.1.4 along with the ions that they produce.

Sodium hydroxide (NaOH) is an ionic compound that is highly soluble, dissociates completely and produces OH^- ions when dissolved. NaOH is therefore considered a strong base. Referring to our solubility rules from Chapter 13, note that all the Group 1 hydroxides and the heavier Group 2 hydroxides are all soluble and dissociate fully in water. They are therefore all listed as examples of strong bases shown in Table 14.1.4.

Interestingly, hydrogen fluoride (HF) does not undergo complete ionisation when dissolved in water, in contrast to the other hydrogen-halides from Group 17 (HCl, HBr and HI). Hydrofluoric acid HF(aq) is a weak acid, undergoing only partial ionisation as shown above. All organic acids are weak acids including those named above, citric acid ($H_3C_6H_5O_7(aq)$), ascorbic acid ($H_2C_6H_6O_6(aq)$) and ethanoic acid ($HC_2H_3O_2(aq)$) as well as the inorganic acids nitrous acid ($HNO_2(aq)$) and cyanic acid (HCN(aq)).

TABLE 14.1.4 Strong acids and strong bases

Acid name	Formula	Ions	Base name	Formula	Ions
hydrochloric acid	HCl	H^+ / Cl^-	lithium hydroxide	LiOH	Li^+ / OH^-
hydrobromic acid	HBr	H^+ / Br^-	sodium hydroxide	NaOH	Na^+ / OH^-
hydroiodic acid	HI	H^+ / I^-	potassium hydroxide	KOH	K^+ / OH^-
nitric acid	HNO_3	H^+ / NO_3^-	rubidium hydroxide	RbOH	Rb^+ / OH^-
chloric acid	$HClO_3$	H^+ / ClO_3^-	caesium hydroxide	CsOH	Cs^+ / OH^-
perchloric acid	$HClO_4$	H^+ / ClO_4^-	calcium hydroxide	$Ca(OH)_2$	Ca^{2+} / $2OH^-$
sulfuric acid	H_2SO_4	H^+ / HSO_4^-	strontium hydroxide	$Sr(OH)_2$	Sr^{2+} / $2OH^-$
			barium hydroxide	$Ba(OH)_2$	Ba^{2+} / $2OH^-$

Ammonia (NH_3) is the most common weak base that is presented in chemistry studies. Weak bases are generally formed from molecular compounds. When dissolved in water, NH_3 molecules react with water molecules to produce OH^- ions. The production of OH^- ions defines ammonia as a base; however, it is considered a weak base since complete ionisation does not occur.

$$NH_3(g) + H_2O(l) \rightleftharpoons NH_4^+(aq) + OH^-(aq)$$

Acid–base strength versus acid–base concentration

Confusion sometimes arises between the strength of an acid (or base) and its **concentration**. A common misconception is that a solution of acid with a high concentration (i.e. a **concentrated solution**) is a strong acid, or that a very low concentration of acid (i.e. a **dilute solution**) is a weak acid. This is not true.

The strength of an acid (or base) is only determined by the extent of ionisation/dissociation and not by its concentration. A strong acid exists almost exclusively as ions when it is dissolved in water, irrespective of its concentration. For example, a hydrochloric acid solution, HCl(aq), with a low concentration of 0.00001 M, is still a solution of a strong acid (i.e. a strong acid in a dilute solution). Conversely, a hydrofluoric acid solution, HF(aq), with a high concentration of 5.0 mol L^{-1} is still a solution of a weak acid (i.e. a weak acid in a concentrated solution).

The same applies to strong bases and weak bases—the strength of a base is only determined by the extent of dissociation or ionisation and not by its concentration.

14.1 Review

SUMMARY

- An Arrhenius acid ionises in water to produce hydrogen ions ($H^+(aq)$). These ions then immediately react with water molecules to form the hydronium ion ($H_3O^+(aq)$).
- In these ionisation reactions, a molecular substance reacts with a solvent such as water to form ions in solution.
- The common properties of acids are due to their ability to form the hydrogen ion, H^+, in solution.
- An Arrhenius base dissociates in water, producing hydroxide ions, OH^-.
- In a dissociation reaction, positive and negative ions separate from an ionic lattice.
- The common properties of bases are due to the presence of the hydroxide ion, OH^-, in solution.
- A hydrogen ion (proton) in solution can be represented by the hydronium ion, $H_3O^+(aq)$, or simply as $H^+(aq)$.
- Acids and bases form electrolyte solutions, which can sustain an electrical current.
- Acids and bases can be characterised as either strong or weak, depending on the extent of dissociation/ionisation.
- The stronger an Arrhenius acid, the more easily it ionises to form the H^+ ion in solution. The stronger an Arrhenius base, the more easily it dissociates to form the hydroxide ion in solution.
- The strength of an acid or base is independent of its concentration.

KEY QUESTIONS

Describe

1 List two common acids and two common bases found in your home.

2 Use the Arrhenius model of acids and bases to identify the ions formed when the following dissociate in water.

a potassium hydroxide

b ethanoic acid

c sulfuric acid

3 List examples of the following using their chemical name and chemical formula:

a two strong acids

b two strong bases

c one weak acid

d one weak base

Apply

4 Use suitable examples to explain the difference between a strong acid and a weak acid.

5 Explain why an aqueous solution of table salt (NaCl) produces an electrically conducting solution, whereas a solution of table sugar ($C_{12}H_{22}O_{11}$) does not.

6 Differentiate, using examples, between an Arrhenius acid and an Arrhenius base.

7 Explain why a very dilute solution (low concentration) of HNO_3 is considered a strong acid.

Analyse

8 Determine some of the limitations of the Arrhenius model of acids and bases using an example in your answer.

9 Two acids (A and B) are prepared with a concentration of 1.0 M ($mol\,L^{-1}$). Acid A produces a solution with a relatively high electrical conductivity. Acid B produces a solution with a relatively low electrical conductivity. Assess the relative strengths of acids A and B and use your understanding of Arrhenius acids to explain your answer.

14.2 pH: a convenient way to measure acidity

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- relate the pH of a solution to the concentration of hydrogen ions within the solution and recognise this as a logarithmic relationship
- compare the pH values for common acids and bases.

In Module 14.1, you learnt that the Arrhenius theory defines acids as substances that ionise in water to produce hydrogen ions. Conversely, the Arrhenius model also defines bases as substances that dissociate in water to produce hydroxide ions. In this module you will learn about the pH scale, which is a measure of acidity/basicity. You will also learn about the relationship between the concentration of hydronium and hydroxide ions in different solutions. To understand these concepts, we first need to consider how water can undergo a process of self-ionisation.

SELF-IONISATION OF WATER

In the previous module, you learnt that some molecular compounds can undergo an ionisation process to form ions in solution. Pure water is a molecular compound that undergoes a **self-ionisation** process, to a very small extent. In this reaction, water behaves as both a very **weak acid** and as a very **weak base**, producing one **hydronium ion** (H_3O^+) for every one hydroxide ion (OH^-). Because water behaves as both a weak acid and a weak base, we say it displays **amphiprotic** properties.

Water molecules can react with each other as represented by the equation:

$$H_2O(l) + H_2O(l) \rightleftharpoons H_3O^+(aq) + OH^-(aq)$$

The production of the H_3O^+ ion and OH^- ion within this reaction can be seen in Figure 14.2.1.

FIGURE 14.2.1 The self-ionisation of water molecules

IONIC PRODUCT OF WATER

When water undergoes self-ionisation, the concentration of hydronium and hydroxide ions is very low. In pure water at 25°C, the H_3O^+ and OH^- concentrations are each 10^{-7} M. For each H_3O^+ ion present in a glass of water, there are 560 million H_2O molecules!

Experimental evidence shows that all aqueous solutions contain both H_3O^+ and OH^- ions, and that the product of their molar concentrations, $[H_3O^+][OH^-]$, is always 1.00×10^{-14} at 25°C. If either $[H_3O^+]$ or $[OH^-]$ in an aqueous solution increases, then the concentration of the other must decrease proportionally.

In solutions of acidic substances, H_3O^+ ions are formed by an ionisation reaction of the acid with water, as well as from self-ionisation of water. So the concentration of H_3O^+ ions will be greater than 10^{-7} M at 25°C. Since the product $[H_3O^+][OH^-]$ remains constant, the concentration of OH^- ions in an **acidic solution** at this temperature must be less than 10^{-7} M.

Square brackets [ ] are typically used to represent the molar concentration (molarity) of a solute in solution.

The opposite is true for **basic solutions**. The concentration of OH^- ions in a basic solution is greater than 10^{-7} M and that of H_3O^+ ions is less than 10^{-7} M.

In summary, at 25°C, the ion concentrations for neutral, acidic and basic solutions are as follows.

- pure water and **neutral solutions**: $[H_3O^+] = [OH^-] = 10^{-7}$ M
- acidic solutions: $[H_3O^+] > 10^{-7}$ M and $[OH^-] < 10^{-7}$ M
- basic solutions: $[H_3O^+] < 10^{-7}$ M and $[OH^-] > 10^{-7}$ M

The higher the concentration of H_3O^+ ions in a solution, the more acidic the solution is.

pH: A CONVENIENT WAY TO MEASURE ACIDITY

Acidity refers to the amount or concentration of acid in a solution. More specifically, it is a measure of the concentration of H_3O^+ ions which, in aqueous solutions, can vary in molar concentration from about 10 M down to 10^{-16} M—an enormous concentration range! The pH scale is a way to conveniently and quantitatively measure this enormous range of acidity.

The pH scale

The range of H_3O^+ concentrations in solutions is so great that a scale was developed specifically to measure acidity. The **pH scale** was first proposed by the Danish scientist Sören Sörenson in 1909 as a way of expressing levels of acidity. The pH of a solution can be represented by the following relationship:

$$pH = -\log_{10} [H_3O^+]$$

Often it is useful to calculate the concentration of hydronium ions, so the equation above can be mathematically rearranged to give:

$$[H_3O^+] = 10^{-pH}$$

The pH scale eliminates the need to write cumbersome powers of 10 when describing hydronium ion concentration. The use of pH greatly simplifies the measurement and calculation of acidity. Since the scale is based upon the negative logarithm of the hydronium ion concentration, the pH of a solution *decreases* as the concentration of hydronium ions *increases*.

Figure 14.2.2 shows a pH meter, which is used to accurately measure the pH of a solution.

FIGURE 14.2.2 A pH meter can be used to measure the acidity of a solution.

Neutral, acidic and basic solutions can be defined in terms of their pH at 25°C.

- Neutral solutions have a pH equal to 7.
- Acidic solutions have a pH less than 7.
- Basic solutions have a pH greater than 7.

On the pH scale, the most highly acidic solutions that you are likely to encounter can have pH values between zero and minus one. Commercial pool acid, for example, is hydrochloric acid with a concentration of about 10 M, which is a pH of −1. The most highly basic solutions that you are likely to encounter can have pH values of about 15. For example, a 5.0 M solution of sodium hydroxide has a pH of 14.7. The pH values of some common substances are provided in Table 14.2.1.

When looking at the pH values in Table 14.2.1, it is important to note that the pH scale is a **logarithmic scale**, not a linear scale. For example, a pH of 1 represents a solution with $[H_3O^+] = 0.1$ M, whereas a pH of 2 represents a solution with $[H_3O^+] = 0.01$ M, which is ten times less! This ten-fold decrease in $[H_3O^+]$ for every unit increase in pH is numerically highlighted in the right-hand column of Table 14.2.1.

i The pH scale is a logarithmic scale. For every unit increase in pH, there is a ten-fold decrease in the concentration of hydronium ions in solution.

TABLE 14.2.1 Approximate pH values of some common substances at 25°C

Solution	pH	$[H_3O^+]$ (M)	$[OH^-]$ (M)	$[H_3O^+]$ relative to pure water	Acidic or alkaline?
1.0 M HCl, battery acid	0	1	10^{-14}	10000000	acidic
stomach acid	1	10^{-1}	10^{-13}	1000000	acidic
lemon juice	2	10^{-2}	10^{-12}	100000	acidic
vinegar	3	10^{-3}	10^{-11}	10000	acidic
tomatoes, acid rain	4	10^{-4}	10^{-10}	1000	acidic
black coffee, bananas	5	10^{-5}	10^{-9}	100	acidic
rain water, milk	6	10^{-6}	10^{-8}	10	acidic
pure water	7	10^{-7}	10^{-7}	1	neutral
sea water, eggs	8	10^{-8}	10^{-6}	0.1	alkaline
soap, baking soda	9	10^{-9}	10^{-5}	0.01	alkaline
milk of magnesia	10	10^{-10}	10^{-4}	0.001	alkaline
ammonia cleaning solution	11	10^{-11}	10^{-3}	0.0001	alkaline
chemical hair straightener	12	10^{-12}	10^{-2}	0.00001	alkaline
oven cleaner	13	10^{-13}	10^{-1}	0.000001	alkaline
1.0 M NaOH, drain cleaner	14	10^{-14}	10^{0}	0.0000001	alkaline

The reactions of acids and bases are important in a large variety of everyday applications. The high acidity of gastric juices is essential for protein digestion in the stomach. There is a complex system of pH control in your blood because even small deviations from the normal pH range of 7.35–7.45 for any length of time can lead to serious illness and death.

Acid–base indicators to measure pH

A characteristic property of acids and bases is their ability to change the colour of certain plant extracts. Litmus is a purple dye obtained from lichen. In the presence of acids, litmus turns red. The colouring of rose petals, blackberries and red cabbage is also altered by acids and bases. Such plant extracts are called indicators, or more specifically, acid–base indicators. Each acid–base indicator has a characteristic pH range over which the dye will change colour. Common indicators and their pH ranges can be seen in Figure 14.2.3.

The relationship between pH and hydronium ion concentration is logarithmic. A solution with pH 2 has 10 times the concentration of hydronium ions as a solution with pH 3. The solution of pH 2 also has one-tenth the concentration of hydroxide ions as a solution with pH 3.

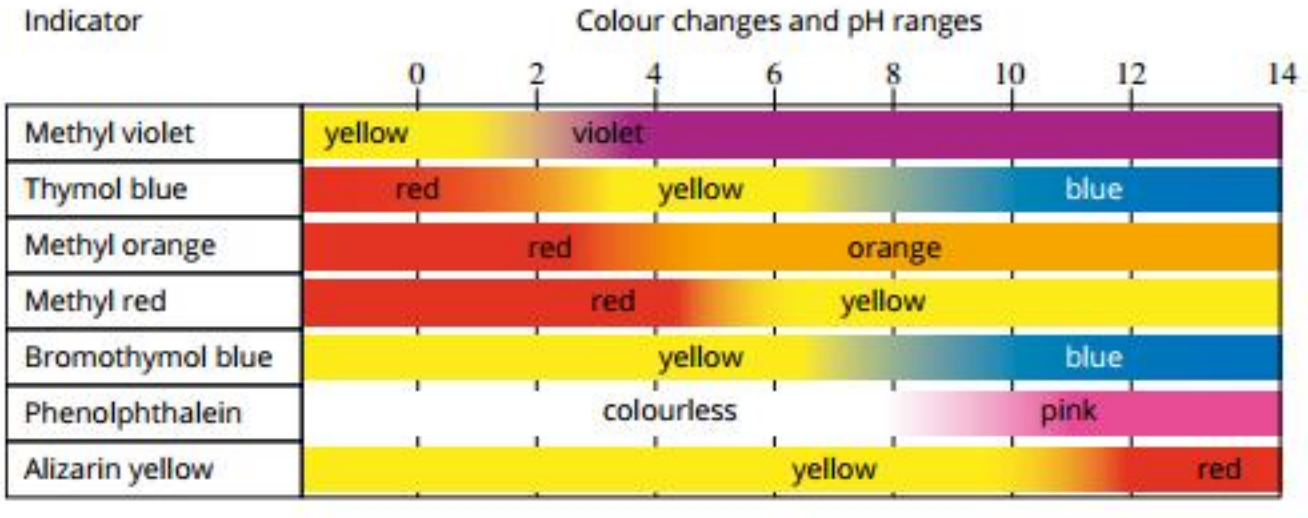


FIGURE 14.2.3 Common indicators and their pH ranges

Universal indicator

Universal indicator (Figure 14.2.4) is widely used to estimate the pH of a solution. It is a mixture of several indicators and changes through a range of colours, from red through yellow, green and blue, to violet. If a more accurate measurement of pH is needed, you can use a pH meter instead of universal indicator.

FIGURE 14.2.4 Universal indicator pH scale. When universal indicator is added to a solution, it changes colour depending on the solution's pH. The tubes contain solutions of pH 0 to 14 from left to right. The green tube (centre) is neutral, pH 7.

14.2 Review

SUMMARY

- Water self-ionises according to the equation: $H_2O(l) + H_2O(l) \rightleftharpoons H_3O^+(aq) + OH^-(aq)$
- The pH of a solution is calculated using the logarithm of $[H_3O^+]$, i.e. $pH = -\log_{10}[H_3O^+]$
- At 25°C, the pH of a neutral solution is 7. The pH of an acidic solution is less than 7 and the pH of a basic solution is greater than 7.
- Indicators are compounds that change colour depending on the relative acidity or basicity of a solution. They are commonly used to provide an indication of the pH of a solution.

KEY QUESTIONS

Describe

1 Write the chemical equation for the self-ionisation reaction of water and identify the products in this chemical process.

2 pH is a measure of what characteristic of aqueous solutions?

3 State the mathematical expression relating pH to the concentration of hydronium ions.

4 Refer to Figure 14.2.3 on page 403 to determine the colour of phenolphthalein indicator in a solution of pH 10.

5 Identify two plant materials whose colour is changed by the addition of an acid or a base.

6 Human blood has a pH of 7.4. Identify blood as acidic, basic or neutral.

Apply

7 The pH of a cola drink is 3 and the pH of black coffee is 5. Distinguish between the two solutions in terms of their acidity. How many times more acidic is one than the other?

8 The pH scale is a logarithmic scale. Explain what this statement means, with reference to examples from Table 14.2.1 on page 403.

Analyse

9 A sample of tomato juice has a pH of 4. Determine the relative concentration of hydrogen ions in tomato juice compared to pure water.

10 When both methyl red and bromothymol blue indicators are added to an industrial effluent, the solution turns yellow. Determine the approximate pH of the effluent.

14.3 Reactions of acids

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand the different reactions involving acids
- predict the products in reactions of acids and other compounds including reactive metals, bases and carbonates
- construct chemical and ionic equations to represent the reactions of acids and bases using correct formulas and symbols.

Acids were originally grouped together because of their similar chemical behaviour. Similarly, all bases share some common properties with respect to their chemical behaviour. Acids and bases react readily with many other chemicals, and some of the early definitions of acids and bases were derived from these reactions.

In this module, you will learn to use the patterns in the reactions of acids to predict the products that are formed.

ACIDS AND REACTIVE METALS

When dilute acids are added to main group metals and some transition metals, bubbles of hydrogen gas are released and a salt is formed. In general, the equation for the reaction is:

$$\text{acid} + \text{reactive metal} \rightarrow \text{salt} + \text{hydrogen gas}$$

Reactive metals include calcium, magnesium, iron and zinc, but *not* copper, silver or gold. For example, the reaction between dilute hydrochloric acid and zinc metal can be seen in Figure 14.3.1 and represented by the equation:

$$2HCl(aq) + Zn(s) \rightarrow ZnCl_2(aq) + H_2(g)$$

This reaction can also be represented by an ionic equation. In an aqueous solution, the hydrochloric acid is ionised and the salt, zinc chloride (a soluble ionic compound), is dissociated. The ionic equation can be determined as shown in the Worked example 14.3.1 on page 408.

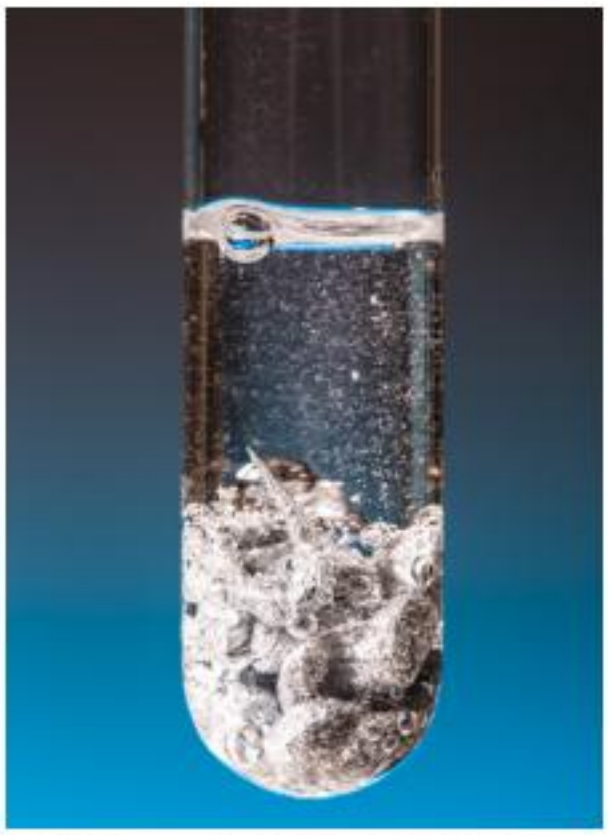


FIGURE 14.3.1 Hydrogen gas is produced from the reaction of zinc with dilute hydrochloric acid.

ACID–BASE NEUTRALISATION REACTIONS

If a solution of a metal hydroxide is added to a solution of an acid (an **acid–base reaction**), the hydroxide ions will react with the hydrogen ions. The acid and base are said to have been **neutralised** at the point when all the hydroxide ions have reacted with all the hydrogen ions, forming water (H_2O).

Soluble metal hydroxides, such as NaOH, dissociate in water to form metal **cations** and hydroxide ions, $OH^-(aq)$. The products of a reaction of an acid with a metal hydroxide are an ionic compound, called a **salt**, and water.

The general rule for the reaction between acids and metal hydroxides can be expressed as:

$$\text{acid} + \text{metal hydroxide} \rightarrow \text{salt} + \text{water}$$

Given that metal hydroxides are bases, we can write a more generalised equation for acid–base neutralisation reactions:

$$\text{acid} + \text{base} \rightarrow \text{salt} + \text{water}$$

For example, solutions of sulfuric acid and sodium hydroxide react to form sodium sulfate (a salt) and water. This can be represented by the full (or overall) equation:

$$H_2SO_4(aq) + 2NaOH(aq) \rightarrow Na_2SO_4(aq) + 2H_2O(l)$$

In water, the sodium and sulfate ions will dissociate, leaving Na^+ and SO_4^{2-} in solution. If water was evaporated from the reaction mixture, solid sodium sulfate would be left behind.

Salts produced in acid–base neutralisation reactions

The salts produced from acid–base neutralisation reactions are ionic compounds in which the positive ion (cation) is derived from the base and the negative ion (anion) is derived from the acid.

Table 14.3.1 lists the names of salts formed from some **neutralisation reactions** of acids with metal hydroxides. Note that the name of the positive ion (from the base) is listed first and the name of the negative ion (from the acid) is listed second.

TABLE 14.3.1 Salts formed from some common acid–base neutralisation reactions

Reactants (acid + metal hydroxide)	Salt formed	Formulas of ions present in the salt solution
hydrochloric acid + potassium hydroxide	potassium chloride (KCl)	$K^+(aq) + Cl^-(aq)$
hydrochloric acid + magnesium hydroxide	magnesium chloride ($MgCl_2$)	$Mg^{2+}(aq) + Cl^-(aq)$
nitric acid + sodium hydroxide	sodium nitrate ($NaNO_3$)	$Na^+(aq) + NO_3^-(aq)$
sulfuric acid + zinc hydroxide	zinc sulfate ($ZnSO_4$)	$Zn^{2+}(aq) + SO_4^{2-}(aq)$
phosphoric acid + potassium hydroxide	potassium phosphate K_3PO_4)	$K^+(aq) + PO_4^{3-}(aq)$
ethanoic acid + calcium hydroxide	calcium ethanoate $Ca(CH_3COO)_2$	$Ca^{2+}(aq) + CH_3COO^-(aq)$

The diagram shown in Figure 14.3.2 represents the ions in solutions of HCl and NaOH when they are mixed in a neutralisation reaction.

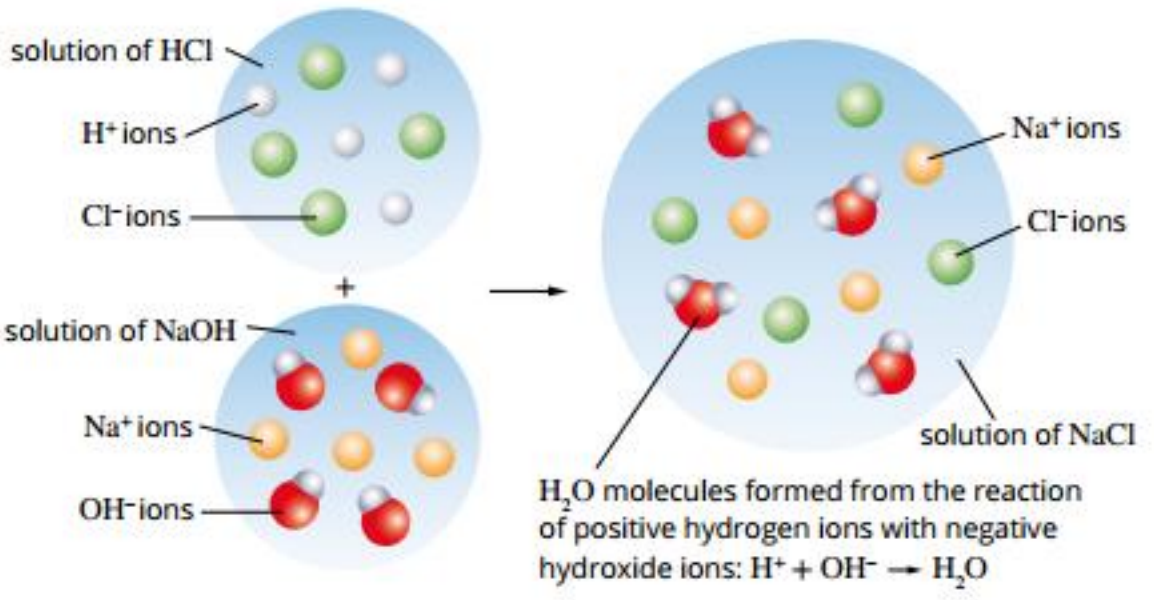


FIGURE 14.3.2 A representation of the reaction between $H^+(aq)$ and $OH^-(aq)$ ions that occurs when solutions of HCl and NaOH are mixed. The products produced are salt solution (NaCl(aq)) and water ($H_2O(l)$).

FIGURE 14.3.3 This statue has been heavily eroded by acid rain, which reacts with carbonate salts in limestone. Acid rain is formed when gases, such as sulfur dioxide and nitrogen oxides, dissolve in water to form acidic solutions.

ACIDS AND METAL CARBONATES

The weathering of buildings and statues (Figure 14.3.3) is due in part to the reaction between acid rain and the carbonate minerals in the stone.

Acids reacting with metal carbonates and metal hydrogen carbonates produce carbon dioxide gas, together with a salt and water. Metal carbonates include sodium carbonate (Na_2CO_3), magnesium carbonate ($MgCO_3$) and calcium carbonate ($CaCO_3$).

The general reaction for metal carbonates with acids can be summarised as:

acid + metal carbonate → salt + water + carbon dioxide

For example, a solution of hydrochloric acid reacting with sodium carbonate solution produces a solution of sodium chloride, water and carbon dioxide gas. The reaction is represented by the equation:

$$2HCl(aq) + Na_2CO_3(aq) \rightarrow 2NaCl(aq) + H_2O(l) + CO_2(g)$$

The reaction between hydrochloric acid and sodium carbonate is represented in Figure 14.3.4.

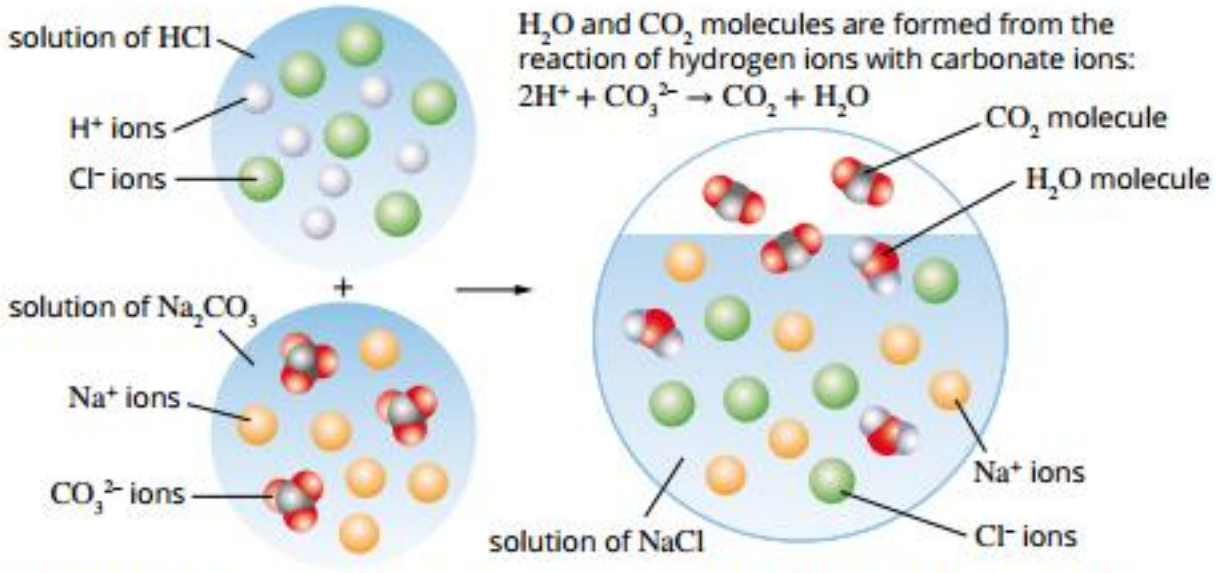


FIGURE 14.3.4 The reaction between solutions of sodium carbonate and hydrochloric acid.

Metal hydrogen carbonates (also known as bicarbonates) include sodium hydrogen carbonate ($NaHCO_3$), potassium hydrogen carbonate ($KHCO_3$) and calcium hydrogen carbonate ($Ca(HCO_3)_2$). Acids added to metal hydrogen carbonates also produce carbon dioxide, together with a salt and water. The general reaction is:

acid + metal hydrogen carbonate → salt + water + carbon dioxide

For example, when solutions of hydrochloric acid and sodium hydrogen carbonate are mixed, the following reaction occurs:

$$HCl(aq) + NaHCO_3(s) \rightarrow NaCl(aq) + H_2O(l) + CO_2(g)$$

Testing for carbonate salts

Acids can be used to detect the presence of carbonate salts. Carbon dioxide is produced when an acid is added to a carbonate.

The **limewater test** is a simple laboratory test used to confirm the presence of carbon dioxide gas. Limewater is a saturated solution of calcium hydroxide ($Ca(OH)_2$). When carbon dioxide is bubbled through this solution, it will turn 'milky' or 'cloudy' in appearance (Figure 14.3.5) due to the precipitation of solid calcium carbonate:

$$Ca(OH)_2(aq) + CO_2(g) \rightarrow CaCO_3(s) + H_2O(l)$$

FIGURE 14.3.5 Limewater test. Carbon dioxide is bubbled through limewater, turning the limewater cloudy.

WRITING IONIC EQUATIONS FOR REACTIONS OF ACIDS

In the sections above, you learnt how acids react with other substances including reactive metals, bases and carbonates. Examples of each of the reactions were represented using chemical equations. They can also be represented using **ionic equations**.

You were introduced to ionic equations when studying precipitation reactions in Chapter 13.

When writing ionic equations, it is important to remember these points.

- Ionic equations are balanced with respect to both the number of atoms of each element and charge.

- **Spectator ions** are ions that are dissolved in the solution and are present as dissolved ions before and after the reaction, but are not involved in the reaction. These are omitted from the ionic equation.
- All strong electrolytes are written as separate dissolved ions in ionic equations. For example, KOH dissolved in water is written as $K^+(aq) + OH^-(aq)$.
- Strong acids ionise in solution and are written as ions; for example, HCl in solution is written as $H^+(aq) + Cl^-(aq)$. We have noted previously that the hydrogen ion can also be represented as the hydronium ion, $H_3O^+(aq)$. You will see in the worked examples below how to write balanced equations using both $H^+(aq)$ and $H_3O^+(aq)$.
- If a reactant or product is a solid, liquid or a gas, it cannot be written as individual (dissolved) ions and it must be fully written in the ionic equation with the (s), (l) or (g) state symbol. For example, water is a covalent molecular substance that does not ionise to any significant extent, so it is written as $H_2O(l)$.
- Salts dissociate in solution to varying degrees depending on their solubility. Weak electrolytes cannot be written as individual ions.

Writing equations and ionic equations for the different reactions will be demonstrated in several worked examples. Worked example 14.3.1 indicates the steps to follow when writing ionic equations for acid–base neutralisation reactions.

In ionic equations, strong electrolytes are written as separate ions in solution; weak electrolytes, solids, liquids and gases are represented with their full chemical equation and state symbol.

Worked example 14.3.1

WRITING AN IONIC EQUATION FOR AN ACID–BASE REACTION

Write an ionic equation for the reaction that occurs when hydrochloric acid is added to sodium hydroxide solution.
A representation of this reaction is shown in Figure 14.3.2 on page 406.

Thinking	Working
What is the general reaction? Identify the products formed.	acid + metal hydroxide → salt + water A solution of sodium chloride and water is formed.
Identify the reactants and products. Indicate the state of each, i.e. (aq), (s), (l) or (g).	Reactants: HCl(aq) is ionised in solution, forming $H^+(aq)$ and $Cl^-(aq)$. NaOH(aq) is dissociated in solution, forming $Na^+(aq)$ and $OH^-(aq)$. Products: Sodium chloride is dissociated and exists as $Na^+(aq)$ and $Cl^-(aq)$. Water is a molecular compound and its formula is $H_2O(l)$.
Write the equation showing all reactants and products, in ionised form where possible. (There is no need to balance the equation yet.)	$H^+(aq) + Cl^-(aq) + Na^+(aq) + OH^-(aq) \rightarrow Na^+(aq) + Cl^-(aq) + H_2O(l)$
Identify the spectator ions: the ions that have an (aq) state both as a reactant and as a product.	$Na^+(aq)$ and $Cl^-(aq)$
Rewrite the equation without the spectator ions. Balance the equation with respect to the number of atoms of each element and charge.	$H^+(aq) + OH^-(aq) \rightarrow H_2O(l)$ Note that if hydrogen ions are represented as hydronium ions, $H_3O^+(aq)$, rather than as $H^+(aq)$, this reaction would be written as: $H_3O^+(aq) + OH^-(aq) \rightarrow 2H_2O(l)$

➤ Try yourself 14.3.1

WRITING AN IONIC EQUATION FOR AN ACID–BASE REACTION

Write an ionic equation for the reaction that occurs when sulfuric acid is added to potassium hydroxide solution.

The reactions between acids and metal carbonates, and reactions between acids and metal hydrogen carbonates, can also be represented as ionic equations by following steps similar to the steps for writing reactions between acids and bases.

Worked example 14.3.2

WRITING IONIC EQUATIONS FOR REACTIONS BETWEEN ACIDS AND METAL CARBONATES

Determine the products formed when a dilute solution of nitric acid is added to solid magnesium carbonate. Write an ionic equation for this reaction.	
Thinking	**Working**
What is the general reaction? Identify the products.	acid + metal carbonate → salt + water + carbon dioxide Products of this reaction are magnesium nitrate in solution, water and carbon dioxide gas.
Identify the reactants and products. Indicate the state of each, i.e. (aq), (s), (l) or (g).	Reactants: Nitric acid is ionised in solution, forming $H^+(aq)$ and $NO_3^-(aq)$ ions. Magnesium carbonate is an ionic solid, $MgCO_3(s)$. Products: Magnesium nitrate is dissociated into $Mg^{2+}(aq)$ and $NO_3^-(aq)$ ions. Water is a molecular compound and its formula is $H_2O(l)$. Carbon dioxide is a molecular compound and its formula is $CO_2(g)$.
Write the equation showing all reactants and products. (There is no need to balance the equation yet.)	$H^+(aq) + NO_3^-(aq) + MgCO_3(s) \rightarrow Mg^{2+}(aq) + NO_3^-(aq) + H_2O(l) + CO_2(g)$
Identify the spectator ions.	$NO_3^-(aq)$
Rewrite the equation without the spectator ions. Balance the equation with respect to the number of atoms of each element and charge.	The equation with spectator ions omitted is: $H^+(aq) + MgCO_3(s) \rightarrow Mg^{2+}(aq) + H_2O(l) + CO_2(g)$ The balanced equation is: $2H^+(aq) + MgCO_3(s) \rightarrow Mg^{2+}(aq) + H_2O(l) + CO_2(g)$ Note that if hydrogen ions are represented as hydronium ions, $H_3O^+(aq)$, rather than as $H^+(aq)$, this reaction would be written as: $2H_3O^+(aq) + MgCO_3(s) \rightarrow Mg^{2+}(aq) + 3H_2O(l) + CO_2(g)$

➤ Try yourself 14.3.2

WRITING IONIC EQUATIONS FOR REACTIONS BETWEEN ACIDS AND METAL CARBONATES

Determine the products formed when a solution of hydrochloric acid is added to a solution of sodium hydrogen carbonate. Write an ionic equation for this reaction.

Worked example 14.3.3

WRITING IONIC EQUATIONS FOR REACTIONS BETWEEN ACIDS AND REACTIVE METALS

Write an ionic equation for the reaction that occurs when dilute hydrochloric acid is added to a sample of zinc metal.	
Thinking	**Working**
What is the general reaction? Identify the products formed.	acid + reactive metal → salt + hydrogen Hydrogen gas and zinc chloride solution are produced.
Identify the reactants and products. Indicate the state of each, i.e. (aq), (s), (l) or (g).	Reactants: Zinc is a solid, Zn(s). Hydrochloric acid is ionised, forming $H^+(aq)$ and $Cl^-(aq)$ ions. Products: Hydrogen gas, $H_2(g)$. Zinc chloride is dissociated into $Zn^{2+}(aq)$ and $Cl^-(aq)$ ions.
Write the equation showing all reactants and products. (There is no need to balance the equation yet.)	$H^+(aq) + Cl^-(aq) + Zn(s) \rightarrow Zn^{2+}(aq) + Cl^-(aq) + H_2(g)$
Identify the spectator ions.	$Cl^-(aq)$
Rewrite the equation without the spectator ions. Balance the equation with respect to the number of atoms of each element and charge.	$H^+(aq) + Zn(s) \rightarrow Zn^{2+}(aq) + H_2(g)$ The balanced ionic equation is: $2H^+(aq) + Zn(s) \rightarrow Zn^{2+}(aq) + H_2(g)$

➤ Try yourself 14.3.3

WRITING IONIC EQUATIONS FOR REACTIONS BETWEEN ACIDS AND REACTIVE METALS

Write an ionic equation for the reaction that occurs when aluminium is added to a dilute solution of hydrochloric acid.

14.3 Review

SUMMARY

- Generalisations can be made about the likely products of reactions involving acids and bases:

  acid + metal hydroxide → salt + water

  acid + metal carbonate → salt + water + carbon dioxide

  acid + metal hydrogen carbonate → salt + water + carbon dioxide

  acid + reactive metal → salt + hydrogen gas
- Each of these reactions can be represented by full and ionic equations.
- Salts dissociate in solution to varying degrees dependent on their solubility. This will then affect whether they are included in full chemical equations or ionic equations. All strong electrolytes will be written as separate dissolved ions in an ionic equation.
- An ionic equation only shows those ions, atoms or molecules that take part in the reaction.
- Spectator ions (ions that do not take part in the reaction) are not included in ionic equations.
- Ionic equations are balanced with respect to both the number of atoms of each element and charge.

KEY QUESTIONS

Describe

1 Complete the following generalised reactions of acids:
- **a** acid + metal hydroxide →
- **b** acid + metal carbonate →
- **c** acid + metal hydrogen carbonate →
- **d** acid + reactive metal →

2 What are spectator ions?

3 Write full chemical equations and ionic equations for the reactions between:
- **a** magnesium and sulfuric acid
- **b** calcium and hydrochloric acid
- **c** zinc and ethanoic acid
- **d** aluminium and nitric acid

4 Name the salt produced in each of the reactions in Question **3**.

5 For each of the following reactions, write:
- **i** a full chemical equation to represent the reaction (remember to include states)
- **ii** an ionic equation

a solid zinc and sulfuric acid

b solid calcium and nitric acid

c solid magnesium hydrogen carbonate and hydrochloric acid

d solid tin(II) carbonate and sulfuric acid

Apply

6 Explain why limewater turns cloudy in the presence of carbon dioxide gas.

7 Differentiate between a full chemical equation and an ionic equation for acid–base neutralisation reactions.

8 Compare and contrast the reactions of sodium carbonate and sodium hydrogen carbonate with hydrochloric acid. (Hint: write balanced chemical equations for both reactions.)

Analyse

9 A student is given two white crystalline substances, sodium chloride and sodium carbonate. Devise a chemical test to differentiate and identify the two salts.

10 Predict the products of the following reactions and write full chemical equations and ionic equations for each.
- **a** Nitric acid solution is mixed with sodium hydroxide solution.
- **b** Blue copper(II) carbonate powder is added to dilute sulfuric acid.

11 Predict the products of the following reactions and write full equations for each.
- **a** Dilute nitric acid is added to a spoon coated with solid zinc.
- **b** Solid bicarbonate of soda (sodium hydrogen carbonate) is mixed with vinegar (a dilute solution of ethanoic acid).

12 Dilute hydrochloric acid is added to a white solid in a test tube. A colourless gas is produced. The gas turns limewater cloudy. Deduce the identity of the white solid.

Chapter review

14

KEY TERMS

acid
acid–base reaction
acidic solution
acidity
alkali
amphiprotic
base
basic solution
concentrated solution
concentration
dilute solution
dissociate
dissociation
electrolyte
hydronium ion
hydroxide ion
indicator
ionic equation
ionisation
ionise
limewater test
logarithmic scale
neutral solution
neutralisation reaction
neutralise
pH scale
salt
self-ionisation
solution
spectator ion
strong acid
strong base
strong electrolyte
weak acid
weak base
weak electrolyte

KEY QUESTIONS

Describe

1 **a** Define a strong acid.
b List the seven common strong acids.

2 **a** Define a strong base.
b List the eight common strong bases.

3 Which of the following is an example of an Arrhenius base?
A HCl
B NaOH
C CH_4
D H_2SO_4

4 Which of the following is an example of an Arrhenius acid?
A NaOH
B HCl
C NH_3
D CH_4

5 What is a common property of Arrhenius bases in aqueous solutions?
A They taste sour.
B They turn litmus paper blue.
C They form hydrogen gas when reacting with metals.
D They decrease the pH of a solution.

6 Determine which one of the following correctly identifies all the products formed when magnesium hydroxide reacts with hydrochloric acid.
A water
B chloride ions
C magnesium ions and chloride ions
D magnesium chloride precipitate
E water, magnesium ions and chloride ions

7 Identify which one of the following equations represents the reaction of a strong acid with water.
A $HNO_3(aq) + H_2O(l) \rightarrow H_3O^+(aq) + NO_3^-(aq)$
B $HF(aq) + H_2O(l) \rightleftharpoons H_3O^+(aq) + F^-(aq)$
C $LiOH(aq) \rightarrow Li^+(aq) + OH^-(aq)$
D $NH_3(aq) + H_2O(l) \rightleftharpoons NH_4^+(aq) + OH^-(aq)$

8 Identify which of the following would be the likely products of the reaction of magnesium carbonate and hydrochloric acid.
A water and magnesium hydroxide
B hydroxide ions and magnesium ions dissociated in water
C carbon dioxide, magnesium ions and water
D magnesium chloride, water and carbon dioxide gas

Apply

9 Which of the following reactions illustrates the behaviour of an Arrhenius acid in water?
A $NH_3 + H_2O \rightarrow NH_4^+ + OH^-$
B $HCl + H_2O \rightarrow H_3O^+ + Cl^-$
C $NaOH + H_2O \rightarrow Na^+ + OH^-$
D $CO_2 + H_2O \rightarrow H_2CO_3$

10 Which of the following statements correctly describes an acid–base neutralization reaction?
A It produces a salt and water.
B It produces an acid and a base.
C It involves the transfer of electrons.
D It always results in a pH of exactly 7.

11 Complete, and balance, the following chemical equations.

a $HNO_3(aq) + KOH(aq) \rightarrow$

b $H_2SO_4(aq) + K_2CO_3(aq) \rightarrow$

c $H_3PO_4(aq) + Ca(HCO_3)_2(s) \rightarrow$

d $HF(aq) + Zn(OH)_2(s) \rightarrow$

12 An acid solution is formed when hydrogen bromide gas is bubbled into water. Represent this ionisation reaction with a balanced full chemical equation.

13 Represent the reaction between an acid, HA, and a soluble metal carbonate, MCO_3, with a balanced ionic equation.

14 Describe the effect of acid rain on limestone.

15 Hydrogen gas is produced when dilute sulfuric acid reacts with aluminium metal.

a Represent this reaction with a balanced full chemical equation.

b Represent this reaction with a balanced ionic equation.

Analyse

16 When a student added phenolphthalein indicator to a clear, aqueous solution, the solution turned pink. What can the student conclude about the aqueous solution?

A The pH is greater than 8 and the solution is acidic.

B The pH is greater than 8 and the solution is basic.

C The pH is less than 8 and the solution is acidic.

D The pH is less than 8 and the solution is basic.

17 What pH would you expect given the following concentrations in aqueous solution:

a $[H_3O^+] = 10^{-6}$ M

b $[OH^-] = 10^{-6}$ M

c $[H_3O^+] = 10^{-11}$ M

d $[OH^-] = 10^{-11}$ M

18 A 0.1 M solution of HCl has a pH of 1.0, whereas a 0.1 M solution of HF has a pH of 2.08. Use your understanding of Arrhenius acids to explain the difference in pH for these two acids.

19 Predict what would happen to the pH of a 1.0 M HCl solution with the addition of 1.0 M NaOH solution.

20 Create a concept map that demonstrates your understanding of the links between the following terms: acid, base, proton, hydrogen ion, hydronium ion.

21 A solution of ethanoic acid has a pH of 2.2. A solution of nitric acid has a pH of 3.6. A student concludes that ethanoic acid is a stronger acid than nitric acid. Assess the student's conclusion.

Interpret

22 Students were given four unlabelled bottles containing different acids, each with a concentration of 0.5 M (mol L^{-1}). Each bottle contained a clear liquid and they all looked identical. They were also given several similar-sized pieces of zinc, a stopwatch and as many test tubes as necessary.

a Design an experiment that could qualitatively demonstrate the strengths of the acids.

b Name the products you would expect from mixing the zinc with an acid.

c Explain how you would determine the relative strengths of the acids and then rank the acids in order from weakest to strongest.

The results one student obtained are shown in the table.

Acid added to the zinc strip	Observations	Time taken for reaction to go to completion (s)
A		342
B		22
C		65
D		178

d Predict the strongest acid, based on the results above.

e Complete the table with the observations you might expect to see from this experiment.

f Judge and rank the acids in order from weakest to strongest acid.

g Propose a list of possible acids that could have been used in this experiment.

Data analysis

DATA SET 1

The information below applies to Questions 1–5.

The electrical conductivity of two acid solutions was measured at various concentrations. The data are tabulated and graphed as shown below.

TABLE 1 Electrical conductivity of two acid solutions at varying concentrations

	Acid A		Acid B	
Concentration ($mg\,L^{-1}$)	**Concentration (mM)**	**Conductivity (µS/cm)**	**Concentration (mM)**	**Conductivity (µS/cm)**
1.00	0.0274	11.7	0.0500	10.0
3.00	0.0822	35.0	0.150	30.1
10.0	0.274	116	0.500	99.2
30.0	0.822	341	1.50	291
100	2.74	1140	5.00	631

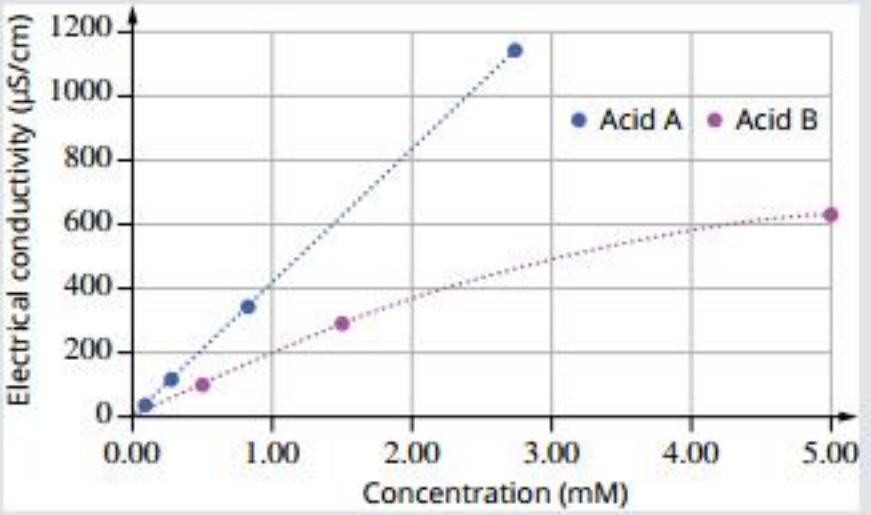


FIGURE 1 Electrical conductivity of two acid solutions at varying concentrations

Question 1 (1 mark)
Use the table and/or graph above to **identify** the unit for electrical conductivity. Write the unit in words and using symbols. Note: the SI unit for electrical conductance is the siemens (S).

Question 2 (2 marks)
There are two different units for concentration shown in the table above: $mg\,L^{-1}$ (milligrams per litre) and mM (millimoles per litre, or millimolar). Use the concentration data in the table to **calculate** the molar mass of acid A.

Question 3 (1 mark)
Interpolate the conductivity of both acids at concentration of 1.00 mM.

Question 4 (3 marks)
Compare the shapes of the curves in the graph above. In your answer, include a similarity, a difference, and an explanation of the significance.

Question 5 (3 marks)
Draw a conclusion about the relative strengths of both acids. **Justify** your answer.

CHAPTER

15 Rates of chemical reactions

Chemical reactions occur at many different rates. The explosion of gunpowder and the combustion of petrol in a car's engine occur very quickly. On the other hand, the weathering of buildings, the ripening of fruit and the rusting of iron all occur quite slowly.

During chemical reactions, particles such as atoms, molecules and ions collide with each other and undergo a rearrangement to produce new substances. It is important to appreciate that collisions between reactant particles do not always result in a chemical reaction. For example, while a car's fuel tank is being filled with petrol, the hydrocarbon molecules in the fuel are colliding with oxygen molecules in the air without a reaction occurring.

By the end of this chapter, you will understand how rates of chemical reactions can be measured and their rates calculated using measurements of changes in the amount of reactants or products. You will also be able to describe how varying the conditions of chemical reactions can affect the rate of a reaction.

Using collision theory, you will learn to predict and explain the effects of concentration of reactants, temperature, surface area, gas pressure and the presence of a catalyst on the rate of chemical reactions.

Enthalpy diagrams, which you used when you studied energy changes in chemical reactions, will be further used to represent energy characteristics of a reaction such as ΔH (enthalpy of reaction) and E_a (activation energy).

Syllabus subject matter

Topic 3 • Rates of chemical reactions

RATES OF REACTIONS

- Explain how temperature, surface area, pressure (gaseous systems), concentration and the presence of a catalyst can affect the rate of the reaction. **15.1, 15.3**
- Apply the collision theory to determine the effect of concentration, temperature, pressure and surface area on the rate of chemical reactions. **15.3**
- Sketch Maxwell–Boltzmann distribution curves for reactions with and without catalysts. **15.3**
- Describe activation energy (E_a). **15.3**
- Explain the relationship between the strength and number of the existing chemical bonds, the magnitude of the activation energy and the rate of a chemical reaction. **15.3**
- Sketch energy profile diagrams for reactions with and without catalysts. **15.3, 15.4**
- Analyse energy profile diagrams for reactions with and without catalysts, to determine the enthalpy change and activation energy. **15.4**

- Explain how catalysts affect the rate of a chemical reaction. **15.4**
- Calculate the rate of chemical reactions by measuring the rate of formation of products or the depletion of reactants. Formula:

$$\text{rate of reaction} = \frac{\text{increase in product concentration } (\Delta[P])}{\text{time taken}} \text{ or}$$

$$\frac{\text{decrease in reactant concentration } (-\Delta[R])}{\text{time taken}} \textbf{ 15.2}$$

- Analyse data and graphical representations of relative changes in the concentration, volume and mass against time to determine rate of reaction. (Order of reaction is not required.) **15.2**

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15.1 Investigating changes to the rates of chemical reactions

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- understand that chemical reactions can occur at significantly different rates
- identify the five major factors that affect the rate of chemical reactions: surface area of solid reactants; concentration of reactants in a solution; gas pressure for reactants in the gaseous state; temperature; and the presence of catalysts.

FIGURE 15.1.1 How quickly do the chemical reactions involved in baking occur?

The time it takes for a chocolate cake to cook in the oven (Figure 15.1.1) and the time taken for a fibreglass patch on a surfboard to set are related to the rates of chemical reactions.

In this module, you will learn how changes to reaction conditions affect reaction rates.

Chemical reactions are taking place all around us:

- in the soil and rocks beneath our feet
- in the air around and above us
- inside every plant and animal
- in our homes, schools and workplaces.

Some of these reactions are over in a flash. In a car accident, when a car's airbag needs to be inflated, the chemical reaction producing the gas that expands the airbag needs to happen extremely quickly. On the other hand, if the car's painted surface is scratched to expose the metal beneath, the rusting reactions take place at a much slower rate.

FACTORS THAT AFFECT REACTION RATES

Experimental investigations have shown that five main factors can change the rate of a **chemical reaction**:

- **surface area** of solid **reactants**
- **concentration** of reactants in a solution
- gas **pressure**
- temperature
- the presence of **catalysts**.

These factors are first addressed here and fully explained in terms of the collision theory in Module 15.3.

FIGURE 15.1.2 Particle size can be used to control the rate of reaction and create different effects during fireworks displays.

Surface area

The surface area of solid reactants can have a significant effect on reaction rate. Smaller particles have a much larger surface area than the same mass of large particles. As a result, the number of collisions between reacting particles is increased and the reaction rate is increased. Smaller particles react faster.

Manufacturers of fireworks modify the surface area of solid reactants to control the rate at which fuels in the fireworks burn and create different effects (Figure 15.1.2). For example, when very small pieces of aluminium are confined inside the shell, they explode violently; however, if larger pieces of aluminium are used, the reaction is slower and the ejection of the burning metal pieces only creates sparks.

Concentration

The concentration of solutes dissolved in a solution can influence the rate of their reactions; higher concentrations usually lead to increased reaction rates because there are more reactant particles present for a given volume of solution.

Pollutants such as sulfur dioxide and nitrogen dioxide are released by cars and many industrial processes. When these compounds react with rainwater, acids such as sulfurous acid and nitric acid are formed. This causes the rainwater's hydrogen ion concentration to increase significantly and it is called **acid rain**. The increasing acidity of rain over the past 200 years has caused many famous marble buildings and statues to deteriorate much more rapidly due to the reaction between marble and the acids (Figure 15.1.3a). Acid rain also causes metals to oxidise more rapidly (Figure 15.1.3b).

FIGURE 15.1.3 (a) This limestone statue has become pitted in recent years. Limestone (calcium carbonate) reacts more rapidly with the increased concentration of hydrogen ions in rainwater. (b) The oxidation of corrugated iron producing red-coloured iron oxide occurs more rapidly with increased acidity of rainwater.

Pressure

In reactions involving gases, increasing the pressure of the gases increases the rate at which the reaction takes place. Increasing the pressure at constant temperature will result in reactant particles becoming closer together. This will increase the frequency of collisions between gas molecules, and therefore increase the rate of reaction. The pressure of the reacting gas will increase if the amount of gas is increased, the temperature of the gas is increased or the volume of the container is decreased.

For this reason, engineers often employ high gas pressures in their design of chemical processes that use gaseous-state reactions. An example is the production of ammonia gas by reacting hydrogen gas and nitrogen gas. Increasing the pressure ensures a faster rate of reaction.

FIGURE 15.1.4 Food is stored at low temperatures in a refrigerator to slow down the rate of reactions that cause food spoilage.

Temperature

As every cook knows, the temperature of an oven affects the rate of the chemical reactions during baking. The higher the temperature, the more rapidly the reactions occur, as most molecules in the baking mixture are moving more rapidly.

On the other hand, in hot weather, it is wise to store fruit and vegetables in the refrigerator so that the chemical reactions that cause them to overripen and then spoil will be slowed down at the lower temperatures (Figure 15.1.4).

Catalysts

Some chemical reactions occur much more rapidly if another substance is added to the reaction mixture. Such substances are called catalysts. Catalysts of various types allow the reaction to follow a more energetically favourable pathway but, themselves, undergo no overall chemical change during the reaction.

For example, if you chew a piece of dry biscuit or bread for several minutes, you may notice it tasting much sweeter. This happens because there is a catalyst present in your saliva that speeds up the breakdown of starch into sweet-tasting sugars.

In the following modules, you will learn how each of these factors can cause these changes in reaction rate.

15.1 Review

SUMMARY

- Rates of chemical reactions vary widely and are affected by a number of experimental factors. The rate of a reaction may be increased by:
  - increasing the surface area of solid reactants
  - increasing the concentration of a reactant in solution
  - increasing the pressure of a gaseous reactant
  - increasing temperature
  - adding a catalyst.

KEY QUESTIONS

Describe

1 List the five experimental variables or factors that affect the rates of chemical reactions.

2 Identify the correct response in the statements about the four main ways in which reaction rates can be increased.

a *increasing/decreasing* surface area of solid reactants

b *increasing/decreasing* the temperature of a reaction mixture

c *increasing/decreasing* the concentration of a reactant in solution

d *increasing/decreasing* the pressure of gaseous reactants

3 State the action of a catalyst.

4 True or False? The rates of chemical reactions can vary from milliseconds to years.

Apply

5 For each of the following, determine whether the proposed change to experimental conditions will increase or decrease the rate of reaction between zinc metal and dilute hydrochloric acid.

a increasing the temperature of the hydrochloric acid

b decreasing the size of the pieces of zinc (while keeping the total mass the same)

c decreasing the concentration of the hydrochloric acid

6 Explain why milk kept in the fridge is able to stay fresh for long periods of time but will quickly spoil at room temperature.

Analyse

7 Commercial epoxy glues consist of two viscous solutions: the epoxy resin and the hardener. The rate of hardening of epoxy glues depends on the amount of hardener that is mixed with the resin. Identify which of the five factors affecting rates of reaction this observation illustrates.

8 Suggest how you could increase the rate of reaction of:

a wood burning on a camp fire

b a cake cooking in an oven

9 Calcium hydroxide (slaked lime) is produced by the hydrolysis of solid calcium oxide (quick lime). When reacting the calcium oxide with water, the following actions were used to increase the rate:

a converting the calcium oxide pieces into a powder

b stirring the quick lime and water reaction mixture

Explain these processes.

10 In medical situations, oxygen gas is provided for treatment. Describe a possible hazard for this environment.

15.2 Quantifying rates of chemical reactions

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- define the rate of a chemical reaction
- analyse changes to reaction rate using data and graphical representations of experimental parameters (concentration, mass, volume) against time
- calculate the average rates of chemical reactions in terms of the disappearance of a reactant or the appearance of a product using

$$\text{rate of reaction} = \frac{\text{increase in product concentration } (\Delta[\text{P}])}{\text{time taken}} \text{ and}$$

$$\text{rate of reaction} = \frac{\text{decrease in reactant concentration } (-\Delta[\text{R}])}{\text{time taken}}$$

- differentiate between average rate, instantaneous rate and initial rate of reaction
- understand the relationship between reaction rate and the stoichiometry of a chemical reaction.

The **rate of reaction** is defined as the change in concentration of a reactant or product per unit time. The usual unit for the rate of reaction is M s^{-1}. To experimentally determine the rate of reaction, you need to measure how much of a reactant is being used up or how much of a product is being formed in a given time period.

In the example shown in Figure 15.2.1, the volume of carbon dioxide produced in the reaction between marble chips and hydrochloric acid is recorded. The experiment was performed twice using the same amount of acid and marble, first with large marble chips and then with small marble chips.

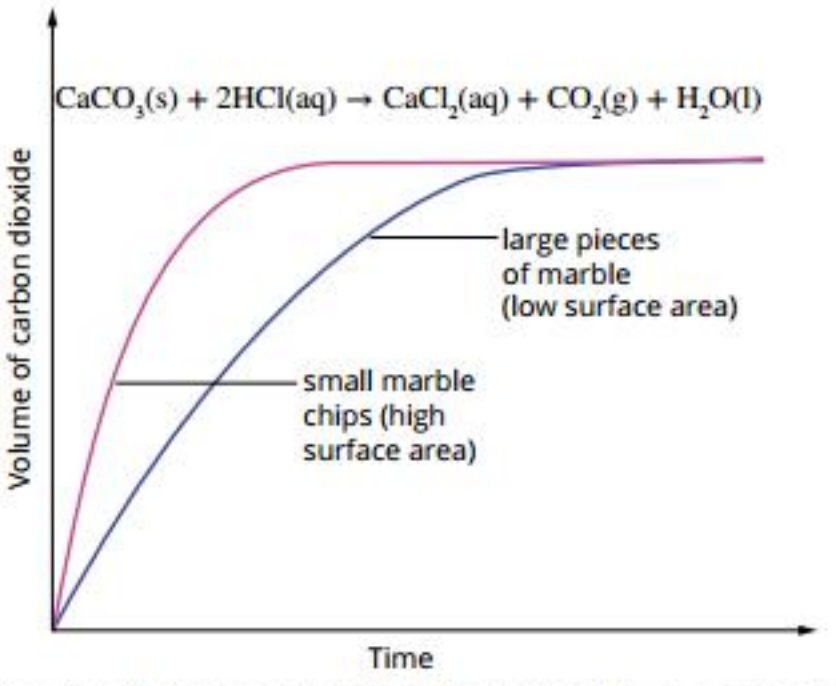

$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$
Volume of carbon dioxide
large pieces of marble (low surface area)
small marble chips (high surface area)
Time

FIGURE 15.2.1 As carbon dioxide is produced from the reaction between marble chips and hydrochloric acid, it is collected in a gas syringe and its volume is recorded. Large and small marble chips are compared.

The steeper slope of the graph with small marble chips indicates that the rate of production of carbon dioxide gas is faster with the marble chips that have a larger surface area.

$$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$$

Mass changes, concentration changes, colour changes and pH changes can also be used to follow the rates of reactions. For example, in the reaction shown in Figure 15.2.1 above, the rate of reaction of $CaCO_3$ with HCl is analysed using a graph of volume of CO_2 produced over time. Alternatively, the rate of this reaction could be determined by following the change in pH as the hydrochloric acid is consumed or the change in mass of the reaction mixture as marble chips are consumed and gas is lost during the reaction.

MEASURING RATES OF REACTION EXPERIMENTALLY

Consider the simplest hypothetical chemical reaction where a single reactant (A) is transformed into a single product (B) represented by the following chemical equation:

$$A \rightarrow B$$

It is important to note that the following discussion relates to the case of this simple hypothetical reaction where the stoichiometric coefficients of the reactants and products are both one. A more complex reaction, in which stoichiometric coefficients are greater than one, is explained later in this module.

The chemical equation above tells us that as reactant A is being consumed, product B is being produced. It therefore follows that as the concentration of A decreases with time, the concentration of B increases with time. The course of this reaction can be followed using **concentration–time curves** (Figure 15.2.2), which show how the concentrations of both A and B change with time and during the course of the chemical reaction.

Closer examination of Figure 15.2.2 shows that the initial slopes of both curves (at time $t = 0$) are quite steep compared to the slopes at later times. This indicates that the reaction is relatively fast at the beginning and slows down with time—a common feature of most chemical reactions.

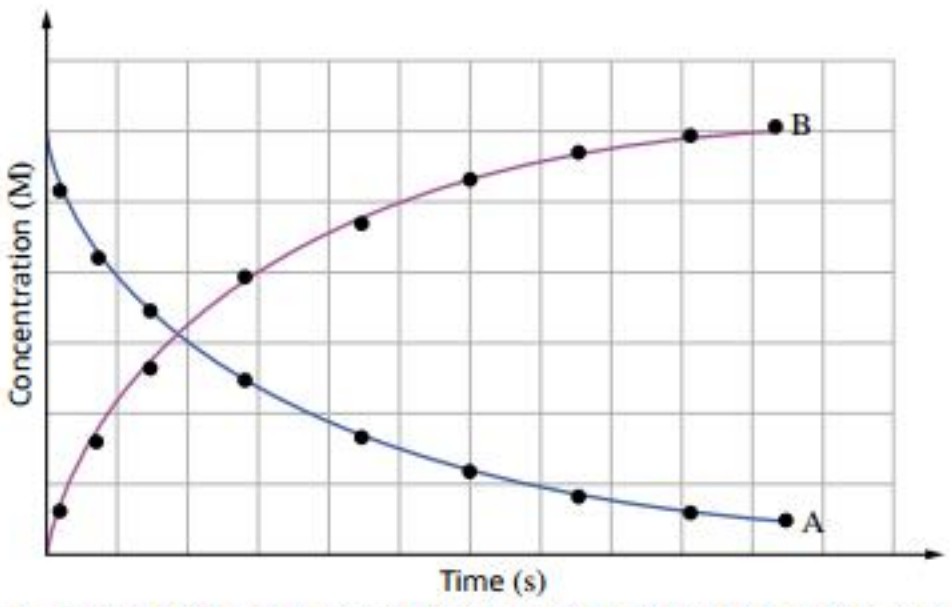


FIGURE 15.2.2 Concentration–time curves showing the changes in concentration over time for the reactant (A) and product (B) for the hypothetical reaction A → B.

Average rate of reaction

The slope of the line between any two points along a concentration–time curve is used to calculate the **average rate of reaction** for that time period. The calculation uses the gradient formula $\frac{\text{rise}}{\text{run}}$ and can use either the rate of disappearance of a reactant or the rate of appearance of a product.

Square brackets are used around chemical formulas to refer to the concentration of that substance.

The rate of reaction is defined as the change in concentration of a reactant or product per unit time. It can be calculated using the rate of disappearance of a reactant or the rate of appearance of a product:

$$\text{rate of reaction} = \frac{\text{decrease in reactant concentration}\left(-\Delta[\text{R}]\right)}{\text{time taken}}$$

or

$$\text{rate of reaction} = \frac{\text{increase in product concentration}\left(\Delta[\text{P}]\right)}{\text{time taken}}$$

Both are equally valid ways of quantifying the rate of reaction and both can be represented mathematically by the following expressions relating to the data in Figure 15.2.2 on page 421:

$$\text{Rate of disappearance of A} = -\frac{\text{change in concentration of reactant A}}{\text{change in time}} = -\frac{\Delta[\text{A}]}{\Delta t}$$

$$\text{Rate of appearance of B} = \frac{\text{change in concentration of product B}}{\text{change in time}} = \frac{\Delta[\text{B}]}{\Delta t}$$

Note that in these mathematical expressions, the 'Δ' sign means 'a change in' and square brackets [ ] means 'concentration of'. You will also note the use of the negative sign in the rate expression for reactant A. Reaction rates are always reported as positive values but since the concentration of a reactant always decreases with time, the value $\frac{\Delta[\text{A}]}{\Delta t}$ will always be a negative number. The negative sign is placed in front of the $\frac{\Delta[\text{A}]}{\Delta t}$ term to ensure the rate will always be reported as a positive value.

The quantities used in calculation of the average rate of formation of the product B are shown in Figure 15.2.3, where Δ[B] = the change in concentration of B (i.e. [B] at t_2 − [B] at t_1) and Δt = change in time ($t_2 - t_1$).

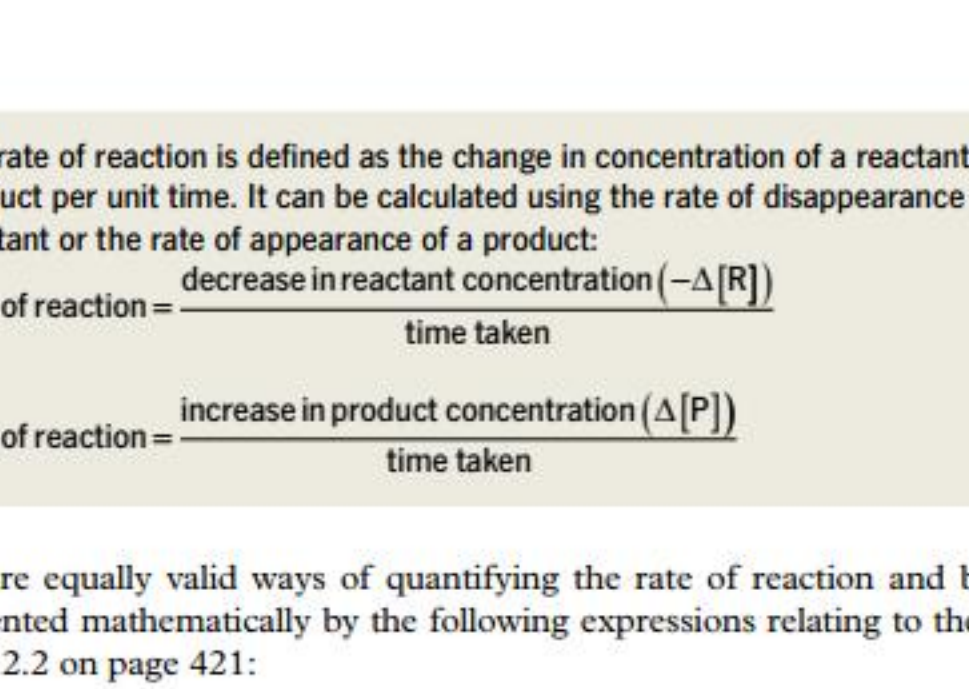


FIGURE 15.2.3 Concentration–time curve for product B in the hypothetical reaction A → B showing that the average rate of reaction between two time points can be calculated from the slope of the line between these two points.

Worked example 15.2.1

CALCULATING AVERAGE RATES OF REACTION

The decomposition of nitrogen dioxide, NO_2, proceeds according to:

$$2NO_2(g) \longrightarrow 2NO(g) + O_2(g)$$

Experimental rate data for this reaction is given below and shows how the concentration of NO_2 decreases with time. Use this data to calculate the average rate of decomposition of NO_2 during the following time intervals.

a $t = 0$ s to $t = 100$ s

b $t = 200$ s to $t = 300$ s

Assume 3 significant figures for all measured values.

Time (s)	$[NO_2]$ (M)
0	0.500
50	0.394
100	0.325
150	0.275
200	0.241
250	0.210
300	0.190

Thinking

The average rate of decomposition of NO_2 is given by:

$$\text{rate of reaction} = \frac{\text{decrease in reactant concentration } (-\Delta[R])}{\text{time taken}}$$

$$\text{Or rate} = -\frac{\Delta[NO_2]}{\Delta t}$$

where: $\Delta [NO_2]$ is the change in concentration of NO_2 during the stipulated time period; and Δt is the time period.

Remember, the negative sign is present in the above expression because the concentration of the reactant is decreasing with time. The negative sign ensures that rate of decomposition will be reported as a positive value.

The 'Δ' quantities are calculated by subtracting an initial quantity from a final quantity, i.e. final concentration minus initial concentration and final time minus initial time.

Working

a In this part of the question, the relevant time period is between zero and 100 s.

$$\Delta NO_2 = [NO_2]_{t=100} - [NO_2]_{t=0}$$
$$= 0.325 - 0.500$$
$$= -0.175\ M$$

$$\Delta t = 100 - 0$$
$$= 100\ s$$

Substituting these two values into the rate equation results in:

average rate between 0 s and 100 s

$$= -\frac{-0.175}{100} = 1.75 \times 10^{-3}\ Ms^{-1}$$

b In this part of the question the relevant time period is between 200 s and 300 s.

$$\Delta NO_2 = [NO_2]_{t=300} - [NO_2]_{t=200}$$
$$= 0.190 - 0.241$$
$$= -0.051\ M$$

$$\Delta t = 300 - 200$$
$$= 100\ s$$

Substituting these two values into the rate equation results in:

average rate between 200 s and 300 s =

$$-\frac{-0.0510}{100} = 5.10 \times 10^{-4}\ Ms^{-1}$$

Note how the rate is quicker in the early part of the reaction compared to later on. This is typical of most chemical reactions.

➤ Try yourself 15.2.1

CALCULATING AVERAGE RATES OF REACTION

Consider the reaction A + B → C. Based on the table of data shown below, calculate the average rate of disappearance of A between 20 s and 40 s in Ms^{-1}.

Time (s)	[A] (M)
0.0	0.224
10.0	0.210
20.0	0.188
30.0	0.173
40.0	0.154

Instantaneous rate of reaction and initial rate of reaction

The average rate of reaction is the most common calculation of reaction rate that you will perform as it uses measured datapoints that you can easily obtain from a graph or table. It provides an average rate during a time period, usually in $M s^{-1}$. Figure 15.2.4 shows the strategy for calculating reaction rate at a specific time point during the chemical reaction (not during a time period). This is aptly called the **instantaneous rate of reaction**. As shown in Figure 15.2.4 the instantaneous rate of reaction is determined by calculating the slope of the tangent to the concentration–time curve at that point. By definition, the line of the tangent should only touch the trend line at a single point—the time point of interest.

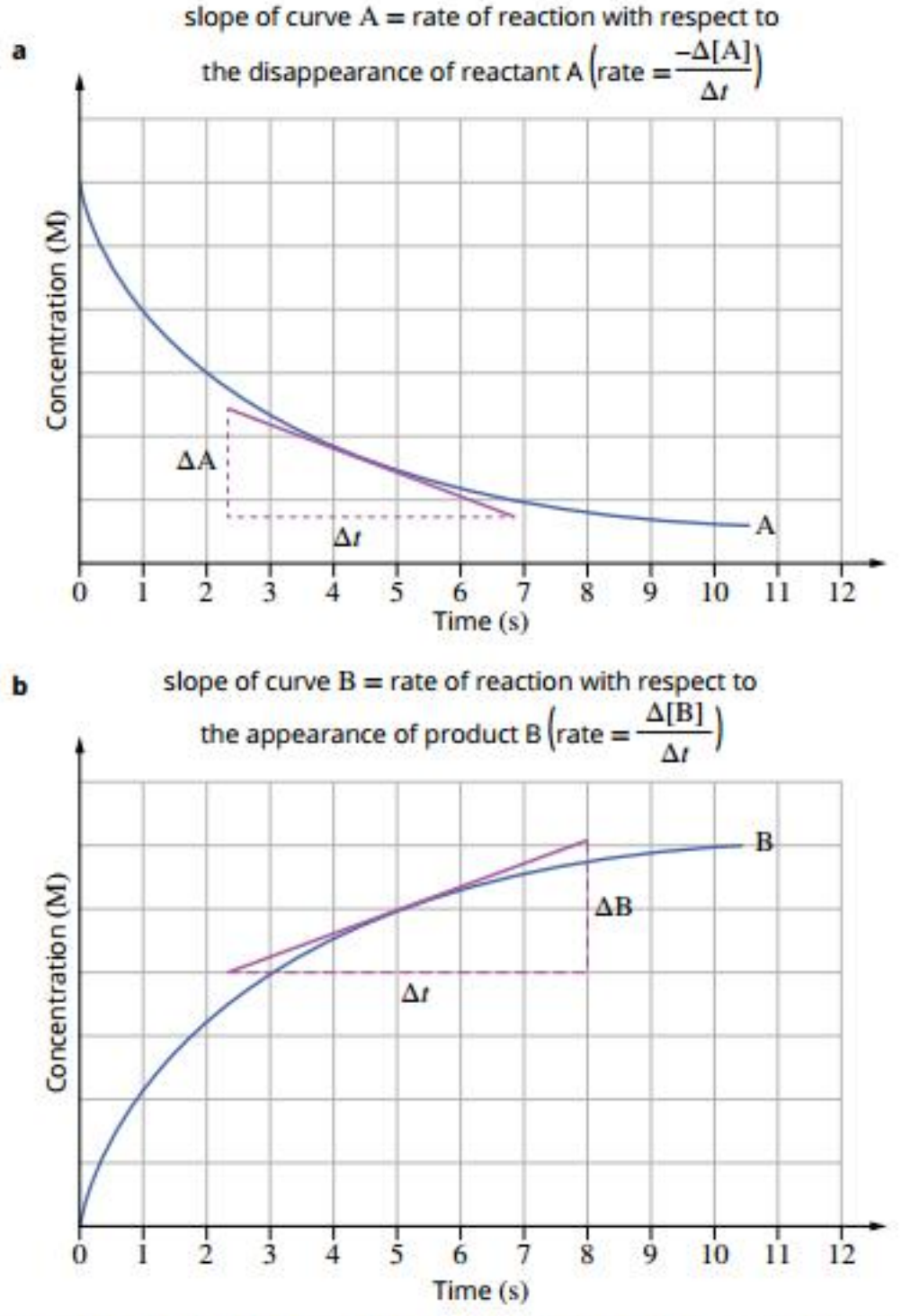

a
slope of curve A = rate of reaction with respect to the disappearance of reactant A $\left(\text{rate} = \frac{-\Delta[A]}{\Delta t}\right)$
Concentration (M)
ΔA
Δt
A
0 1 2 3 4 5 6 7 8 9 10 11 12
Time (s)
b
slope of curve B = rate of reaction with respect to the appearance of product B $\left(\text{rate} = \frac{\Delta[B]}{\Delta t}\right)$
Concentration (M)
B
ΔB
Δt
0 1 2 3 4 5 6 7 8 9 10 11 12
Time (s)

FIGURE 15.2.4 Concentration–time curves for the hypothetical reaction A → B. (a) The slope of the tangent at any point on curve A is equivalent in magnitude to the instantaneous rate of disappearance of reactant A. The rise/run calculation shown provides the instantaneous reaction rate at 4.5 s. (b) The slope of the tangent at any point on curve B is equivalent in magnitude to the instantaneous rate of production of product B. The rise/run calculation shown provides the instantaneous reaction rate at 5.0 s.

The **initial rate of reaction** refers to the instantaneous rate of reaction at time, $t = 0$. Figure 15.2.5 shows that the initial rate of reaction can be calculated by determining the initial slope of a concentration–time curve. Like the instantaneous rate, the initial rate can be calculated using the rate of disappearance of reactant (Figure 15.2.5a) or the rate of appearance of product (Figure 15.2.5b).

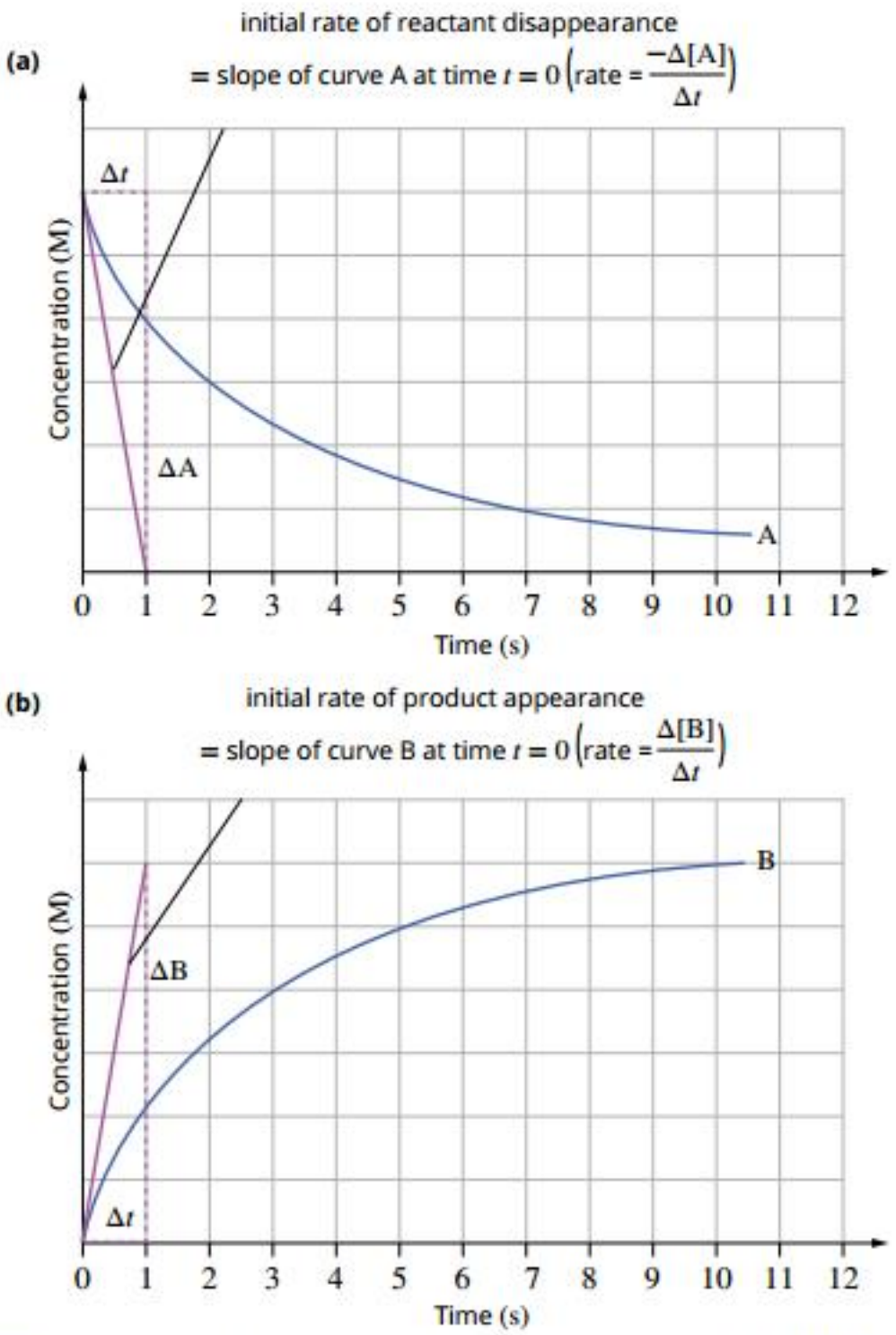

(a)
initial rate of reactant disappearance
= slope of curve A at time $t = 0$ $\left(\text{rate} = \frac{-\Delta[A]}{\Delta t}\right)$
Δt
ΔA
A
Concentration (M)
0 1 2 3 4 5 6 7 8 9 10 11 12
Time (s)
(b)
initial rate of product appearance
= slope of curve B at time $t = 0$ $\left(\text{rate} = \frac{\Delta[B]}{\Delta t}\right)$
B
ΔB
Δt
Concentration (M)
0 1 2 3 4 5 6 7 8 9 10 11 12
Time (s)

FIGURE 15.2.5 Concentration–time curves for the hypothetical reaction A → B. (a) The slope of the tangent at time $t = 0$ on curve A is equivalent in magnitude to the initial rate of reaction. (b) The slope of the tangent at time $t = 0$ on curve B is equivalent in magnitude to the initial rate of reaction.

In practice, measuring the instantaneous rate at any point in time can be difficult for many chemical reactions as it requires the construction of a complete concentration–time curve and the careful drawing of a tangent.

Relationship between reaction rate and stoichiometry

The examples above show how different measures of the rate of a chemical reaction can be calculated for the simple, hypothetical case of a single reactant (A) producing a single product (B). You will now consider a real example of a chemical reaction containing multiple reactants and products where the stoichiometric coefficients take on various values.

The decomposition of dinitrogen pentoxide can be represented by the following chemical equation:

$$2N_2O_5(g) \rightarrow 4NO_2(g) + O_2(g)$$

Reaction rates for this reaction can be expressed in three ways (see below) by considering the rate of disappearance of N_2O_5 as well as the rate of appearance of both NO_2 and O_2.

$$\text{Rate of disappearance of } N_2O_5 = -\frac{\Delta[N_2O_5]}{\Delta t}$$

$$\text{Rate of appearance of } NO_2 = \frac{\Delta[NO_2]}{\Delta t}$$

$$\text{Rate of appearance of } O_2 = \frac{\Delta[O_2]}{\Delta t}$$

Note: the negative sign in front of the $\frac{\Delta[N_2O_5]}{\Delta t}$ term is used because N_2O_5 is a reactant and its concentration decreases with time.

The problem with this approach is that the three expressions for rate are not mathematically equivalent. When you look at the stoichiometric coefficients in the balanced chemical equation, you will note that for every 2 moles of N_2O_5 that is consumed in any time period, 4 moles of NO_2 will be produced. The rate of appearance of NO_2 is therefore twice as great as the rate of disappearance of N_2O_5. Similarly, for every 2 moles of N_2O_5 consumed, only 1 mole of O_2 will be produced in any given time period: the rate of appearance of O_2 is therefore one-half the rate of disappearance of N_2O_5.

As you can see, the rate of disappearance of reactants and the rate of appearance of products are not the same if the stoichiometric coefficients differ. It would be much more meaningful to define the value for the rate of reaction as being the same value regardless of the values of stoichiometric coefficients or whether you monitor the disappearance of reactants or the appearance of products.

To do this, you must take into account the value of the stoichiometric coefficient for each substance in the chemical reaction. In this case, the rate of reaction with respect to each substance in the reaction can be reported as:

$$\text{Rate of reaction} = -\frac{1}{2}\frac{\Delta[N_2O_5]}{\Delta t} = \frac{1}{4}\frac{\Delta[NO_2]}{\Delta t} = \frac{\Delta[O_2]}{\Delta t}$$

By expressing the rate of reaction in this way, each of the three expressions for rate are mathematically equivalent.

In general, for any chemical reaction that takes the form:

$$aA + bB \rightarrow cC + dD$$

where the lower-case letters represent the stoichiometric coefficients for each substance, the rate of reaction can be written as:

$$\text{Rate of reaction} = -\frac{1}{a}\frac{\Delta[A]}{\Delta t} = -\frac{1}{b}\frac{\Delta[B]}{\Delta t} = \frac{1}{c}\frac{\Delta[C]}{\Delta t} = \frac{1}{d}\frac{\Delta[D]}{\Delta t}$$

It is important to understand the difference between the rate of reaction and the rate of disappearance of reactants (or the rate of appearance of products). The rate of a chemical reaction at any point in time has only one value and is independent of the reaction stoichiometry. The rate of disappearance of reactants and the rate of appearance of products will be different to this value if the stoichiometric coefficients are different.

Worked example 15.2.2

REACTION RATE AND STOICHIOMETRY

The decomposition of HI proceeds according to:

$$2HI(g) \rightarrow H_2(g) + I_2(g)$$

a Write an expression for the rate of this chemical reaction showing the relationship between the rate of consumption of HI and the rate of production of both H_2 and I_2.

b Write an expression for the rate of decomposition of HI and show how it differs to the overall rate of reaction expression derived in part **a**.

Thinking	Working
a When writing an expression for the overall rate of a chemical reaction, you have to take into account the stoichiometric coefficients. This is particularly important when the coefficients are different for different substances in the balanced chemical equation. Using the approach outlined above, if the chemical equation takes the form of $aA + bB \rightarrow cC + dD$ the rate of reaction can be written as: $\text{Rate} = -\frac{1}{a}\frac{\Delta[A]}{\Delta t} = -\frac{1}{b}\frac{\Delta[B]}{\Delta t} = \frac{1}{c}\frac{\Delta[C]}{\Delta t} = \frac{1}{d}\frac{\Delta[D]}{\Delta t}$ where the lower-case letters represent the stoichiometric coefficients for each substance. Remember, you need to place a negative sign in front of the expression for any reactants.	**a** In this example the coefficient of HI is 2, while the coefficients of H_2 and I_2 are both 1. By multiplying by the inverse of the stoichiometric coefficients and multiplying the expression for any reactants by –1, the expression for the rate of reaction is $\text{Rate} = -\frac{1}{2}\frac{\Delta[HI]}{\Delta t} = \frac{\Delta[H_2]}{\Delta t} = \frac{\Delta[I_2]}{\Delta t}$ When written like this, the rate equation expression shows how the rate of disappearance of reactants relates to the rate of appearance of the products.
b It is important to understand the difference between the rate of a reaction and the rate of disappearance (or decomposition) of a reactant. The rate of a chemical reaction at any point in time has only one value and is independent of the reaction stoichiometry. The rate of disappearance of reactants and the rate of appearance of products will be different to this value if the stoichiometric coefficients are different.	**b** The expression for the rate of decomposition of HI is given by the change in concentration over time $\text{Rate of decomposition} = -\frac{\Delta[HI]}{\Delta t}$ The expression for the overall rate of reaction needs to take into account the stoichiometric coefficient of HI, i.e. $\text{Rate of reaction} = -\frac{1}{2}\frac{\Delta[HI]}{\Delta t}$ The rate of reaction for this reaction is therefore half of the rate of decomposition of HI.

➤ Try yourself 15.2.2

REACTION RATE AND STOICHIOMETRY

Chloryl fluoride (ClO_2F) is produced from the reaction of fluorine and chlorine dioxide. The chemical equation for this reaction is:

$$F_2(g) + 2ClO_2(g) \rightarrow 2ClO_2F(g)$$

Write an expression for the rate of reaction showing how the rate of formation of ClO_2F is related to the rate of consumption of F_2 and ClO_2.

15.2 Review

SUMMARY

- The rate of a chemical reaction is defined as the change in concentration of a reactant or product per unit time.
- The usual unit for rate of reaction is $M s^{-1}$
- A range of experimental methods can be used to measure the rate of a reaction, including measuring the following at specific time intervals (an example unit of each is shown):
  - mass loss ($g\ s^{-1}$)
  - volume of gas produced ($cm^3\ min^{-1}$)
  - colour change
  - concentration change ($M\ min^{-1}$)
  - pH change ($pH\ s^{-1}$).
- The average rate of a chemical reaction can be determined by examining the rate of disappearance of a reactant (R) or by examining the rate of appearance of a product (P).

$$\text{rate of reaction} = \frac{\text{decrease in reactant concentration } (-\Delta[R])}{\text{time taken}}$$

$$\text{rate of reaction} = \frac{\text{increase in product concentration } (\Delta[P])}{\text{time taken}}$$

- The average rate of reaction is calculated (as shown above) using graphical (concentration–time curve) data or tabulated data and relates to a given time period during the reaction.
- The instantaneous rate of reaction and the initial (instantaneous) rate of reaction are calculated using the gradient of a tangent to the concentration–time curve at a particular time point.
- The rate of change of each chemical species in the reaction is related to stoichiometry. Calculating the rate for the reaction needs to consider the stoichiometric coefficient for the species measured. For the general chemical reaction:

$$aA + bB \rightarrow cC + dD$$

the rate of reaction is equal to any of the following:

$$\text{Rate} = -\frac{1}{a}\frac{\Delta[A]}{\Delta t} = -\frac{1}{b}\frac{\Delta[B]}{\Delta t} = \frac{1}{c}\frac{\Delta[C]}{\Delta t} = \frac{1}{d}\frac{\Delta[D]}{\Delta t}$$

where the lower-case letters represent the stoichiometric coefficients for each substance in the balanced chemical equation.

KEY QUESTIONS

Describe

1 Name the unit for the rate of a chemical reaction.

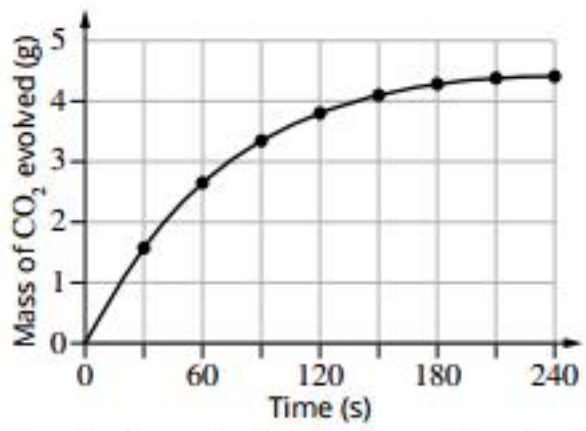
2 List the three different types of reaction rates that can be obtained from the data in a concentration–time curve.

3 Recall the formula for calculating the rate of a reaction when formation of products is measured.

4 Comment on the statement: 'The steepness of the concentration–time graph is greater at the end of the reaction compared to the beginning of the reaction.'

Apply

5 The graph below shows the mass of carbon dioxide gas produced during a 4-minute period of a reaction between marble chips (calcium carbonate) and 1.0 M nitric acid.

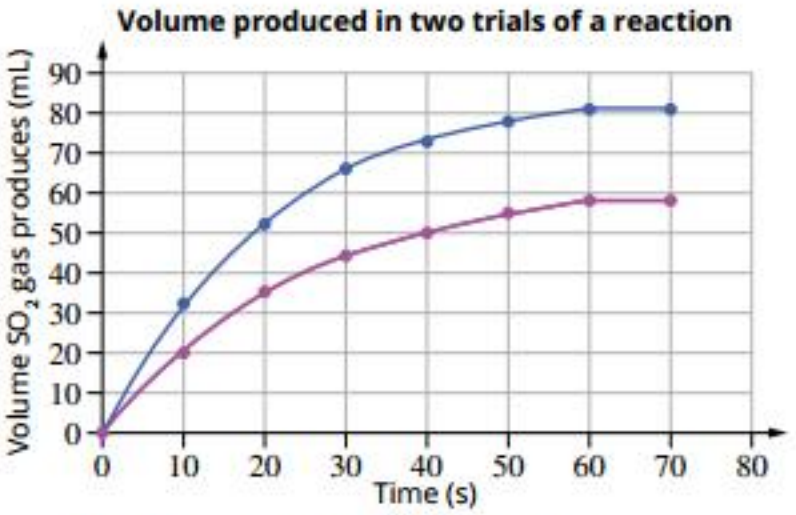


a Write a balanced chemical equation (including state symbols) for this reaction.

b Describe whether the rate of this chemical reaction is increasing or decreasing over time. In your response, refer to gradient(s) shown in the graph. Calculate two values for reaction rate to justify your response.

6 The gas produced from the chemical reaction between hydrochloric acid and sodium thiosulfate (equation shown below) was collected, measured and the data graphed. The graph shows two trials of this reaction conducted using acid solutions of different concentrations.

$$S_2O_3^{2-}(aq) + 2H^+(aq) \rightarrow S(s) + SO_2(g) + H_2O(l)$$



a Identify the reaction which used the lower concentration acid and provide a reason for this.

b Calculate the average rates of each reaction between 0 and 20 seconds.

c Using the information provided about the reactants, products and their states, deduce a further experimental parameter that could be used to measure the rate of this chemical reaction.

Analyse

7 Compare the instantaneous rate of a chemical reaction with the initial rate of a chemical reaction.

8 For the reaction of X and Y (represented by the following chemical equation), distinguish between the rate of consumption of X and the rate of reaction with respect to X.

$$2X + Y \rightarrow Z$$

9 Consider a reaction represented by the following chemical equation:

$$A + B \rightarrow C$$

Based on the concentration time data shown in the table below, calculate the average rate of reaction between each of the two times.

a 0s and 20s

b 20s and 40s

Time (s)	[A] (M)
0.0	0.290
10.0	0.220
20.0	0.178
30.0	0.156
40.0	0.148

10 The following data was obtained for the decomposition of hydrogen peroxide, H_2O_2.

Time (s)	$[H_2O_2]$ (M)
0.0	0.852
10.0	0.636
20.0	0.462
30.0	0.326
40.0	0.218

The balanced chemical equation for this chemical reaction is:

$$2H_2O_2(l) \rightarrow 2H_2O(l) + O_2(g)$$

a Calculate the average rate of decomposition of H_2O_2 between 10.0s and 30.0s.

b Calculate the average rate of reaction between 10.0s and 30.0s.

15.3 Collision theory and factors affecting reaction rate

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- apply collision theory to explain reaction rate by describing that reactant particles need to collide with sufficient energy and with the correct orientation to produce products
  - explain how activation energy is the energy required to break bonds in reactants
  - sketch Maxwell–Boltzmann distribution curves for reactions at different temperatures and reactions with and without catalysts
  - describe how plotting activation energy on a Maxwell–Boltzmann curve indicates the proportion of reacting particles
- differentiate between exothermic and endothermic reactions using changes to enthalpy over time
- sketch and analyse the potential energies of reactants and products on an energy profile diagram and show the effect of a catalyst on the profile
- explain experimental factors that increase the rate and energy of collisions and thereby increase the rate of reaction: surface area of solid reactants; concentration of reactants in a solution; gas pressure for reactants in the gaseous state; temperature; and the presence of a catalyst.

FIGURE 15.3.1 The decomposition of hydrogen peroxide is usually very slow, but the addition of crystals of potassium permanganate results in the rapid evolution of oxygen gas and water vapour.

The chemical equation for a reaction indicates the nature of the reactants and products, but provides no information about the rate at which the reaction proceeds.

Look at the equation for the decomposition of hydrogen peroxide:

$$2H_2O_2(l) \rightarrow 2H_2O(l) + O_2(g)$$

This equation gives no indication about whether the reaction proceeds quickly or slowly; nor can you tell how the products have been formed.

In fact, this reaction normally occurs very slowly, but when a catalyst, such as crystals of potassium permanganate, is added to the hydrogen peroxide solution, the reaction occurs rapidly, producing so much oxygen gas and heat that the reaction mixture foams and some of the liquid water vaporises (Figure 15.3.1).

Chemical reactions occur as a result of collisions between the reacting particles. This idea is part of the **collision theory** of reaction rates, which will be discussed in this module.

COLLISION THEORY AND ACTIVATION ENERGY

During chemical reactions, particles (atoms, molecules or ions) collide and are rearranged to produce new particles. Consider the decomposition reaction of hydrogen peroxide:

$$2H_2O_2(l) \rightarrow 2H_2O(l) + O_2(g)$$

The collision that forms the first step of the reaction occurs between the two hydrogen peroxide molecules. If this collision is to result in the formation of molecules of water and oxygen, the collision must occur in such a way that the covalent bonds in the hydrogen peroxide break. To break bonds in reactants, energy is required. This energy will be greater for reactions where the bond energies (strength of bonds) are greater and where the number of bonds to be broken in the reactants is greater. Bond energy values are provided in the QCAA Formula and Data book. Calculations using these values were described in Chapter 10.

The collision theory of reactions explains why some collisions result in reactions and others do not. According to collision theory, for a reaction to occur, the reactant particles must:

- collide with each other
- collide with sufficient energy to break the bonds within the reactants
- collide with the correct orientation to break the bonds within the reactants and so allow the formation of new products.

If a collision does not meet all of these requirements, then no reaction occurs. In fact, most collisions do not result in a chemical reaction. Collision theory explains why this is the case.

Activation energy

For a reaction to occur between reactant molecules, the molecules must collide with a certain minimum amount of energy so that the bonds in reactants are broken. Unless this minimum amount of energy is met or exceeded, the colliding molecules will rebound and simply move away from each other without reacting. This rebound leaves molecules intact and no reaction occurs.

The minimum energy that a collision must possess for a reaction to occur is called the **activation energy**, E_a. When the energy of a collision is equal to or greater than the activation energy, a reaction can occur.

Activation energy can be represented on an **energy profile diagram** which also indicates if the reaction is **endothermic** or **exothermic**. An energy profile diagram (Figure 15.3.2a, Figure 15.3.2b) represents the potential energy of the system (both reactants and products) over the course of the reaction. These ideas were presented in Chapter 10.

The energy profile diagram for an exothermic combustion reaction like the one shown in Figure 15.3.2a indicates that the enthalpy of the products is always less than the enthalpy of the reactants. Overall, energy is released and so the ΔH value is negative. The energy profile also shows that, even in exothermic reactions, the activation energy must first be absorbed to start the reaction.

The energy profile diagram for an endothermic reaction (Figure 15.3.2b) shows that the enthalpy of the products is greater than the enthalpy of the reactants. Overall, energy is absorbed and so the ΔH value is positive. The energy profile also shows the absorption of the activation energy before the release of energy as bonds form in the products.

Energy profile diagrams for both exothermic and endothermic reactions have a peak that represents the activation energy. This is sometimes referred to as the activation energy barrier and represents the minimum energy that must be absorbed in order to break the bonds of reactants so that a chemical reaction can progress. The activation energy is measured from the energy of the reactants to the top of the peak.

You will recall, from Module 10.2, that an exothermic reaction releases more heat energy during the reaction than it absorbs. An endothermic reaction absorbs more heat energy during the reaction than it releases. This is represented on the diagram as ΔH and is the difference in energy between the reactants and the products.

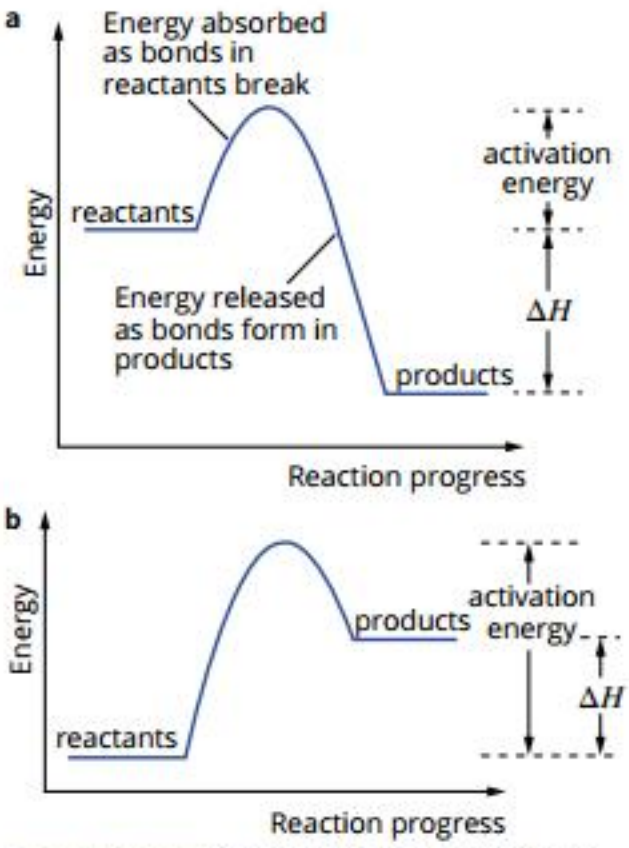


FIGURE 15.3.2 Energy profile diagrams for two reactions (a) small E_a and negative ΔH (b) large E_a and positive ΔH.

Reactant particles must have energy equal to or greater than the activation energy before a reaction can occur.

Transition state

When the activation energy is absorbed, a new arrangement of atoms known as the **transition state** occurs. The transition state occurs at the stage of maximum **potential energy** in the reaction; the activation energy (Figure 15.3.3). Bond breaking and bond forming are both occurring at this stage, and the arrangement of atoms is unstable. The atoms in the transition state rearrange into products as the reaction progresses.

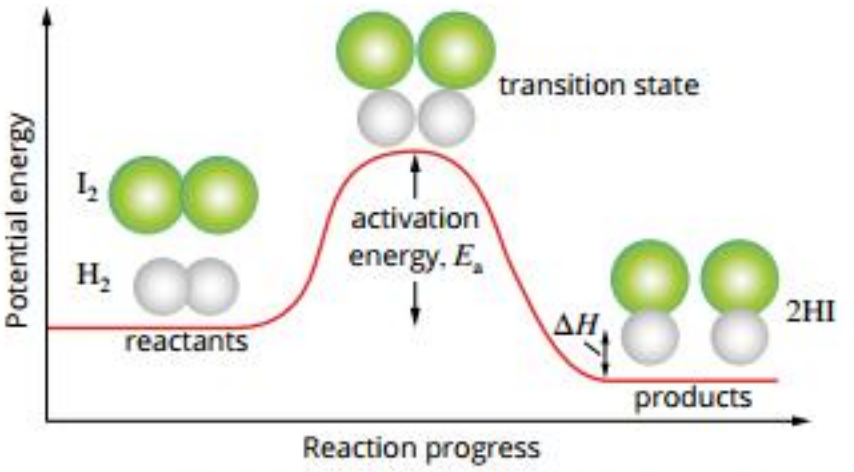


FIGURE 15.3.3 Energy profile diagram for the exothermic reaction $H_2(g) + I_2(g) \rightarrow 2HI(g)$.

Activation energy and reaction rate

The size of the activation energy affects what proportion of collisions results in successful reactions and therefore determines how easy it is for a reaction to occur. For this reason, the reaction rate is dependent upon the activation energy. A chemical reaction with a relatively high activation energy will tend to have a lower reaction rate because many of the reactant particles will not have sufficient energy to exceed the activation energy. Conversely, a chemical reaction with a relatively low activation energy will tend to have a higher reaction rate because many of the reactant particles will have sufficient energy to exceed the activation energy. Figure 15.3.4 represents the energy profile diagrams for two exothermic reactions. While the rate of these reactions will also depend on the energy of the system and the reaction itself, we can deduce that the higher activation energy is likely to present a greater energy barrier (fewer particles will have sufficient energy to overcome E_a) and therefore the reaction rate will likely be slower.

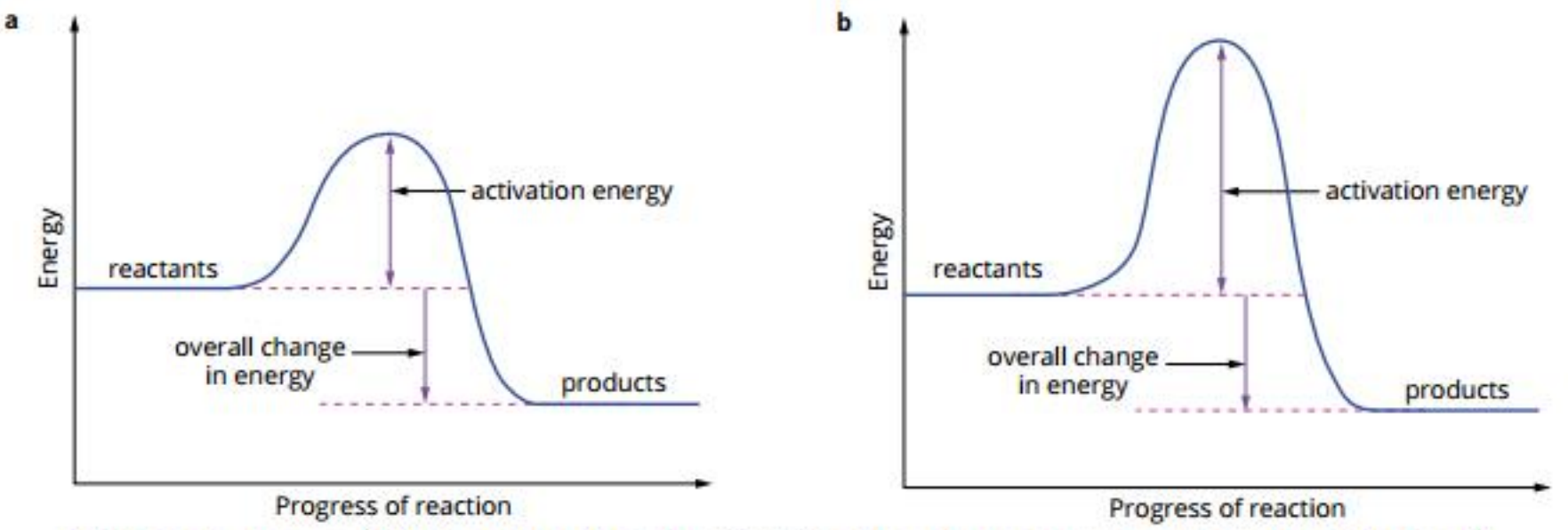


FIGURE 15.3.4 Energy profile for two exothermic reactions. (a) Relatively low activation energy suggests a faster reaction than (b) which has a higher activation energy—fewer particles are likely to have sufficient energy to overcome E_a of the reaction in (b).

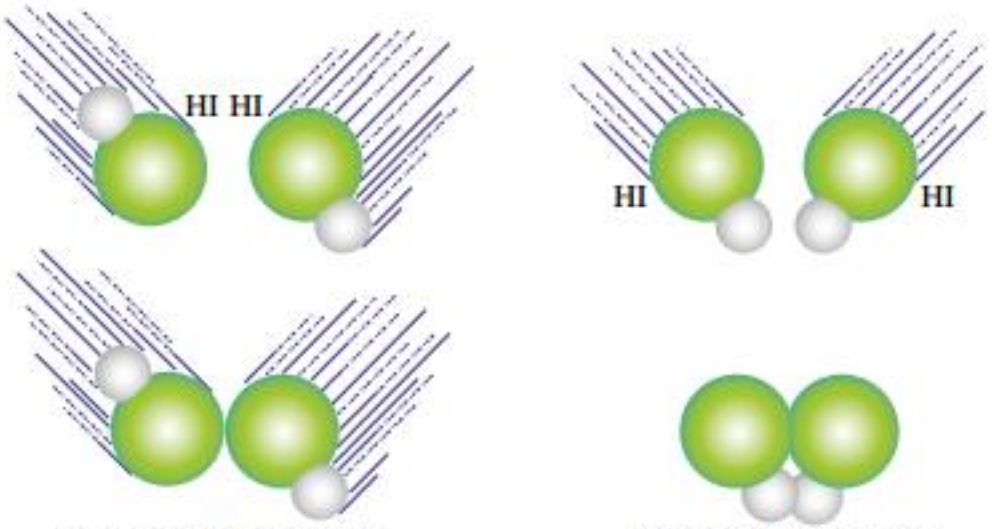
Orientation of colliding molecules

For a reaction to occur, reactants need to collide with enough energy to overcome the activation energy. Reacting molecules must also collide with each other in the correct orientation in such a way that particular bonds in the reactants are broken and new bonds are formed in the products.

Figure 15.3.5 shows the importance of collision orientation. The decomposition of hydrogen iodide gas to produce hydrogen gas and iodine gas can be represented by the following chemical equation:

$$2HI(g) \rightarrow H_2(g) + I_2(g)$$

For this reaction to proceed the two hydrogen iodide molecules must collide with the hydrogen and iodine atoms orientated towards each other, for a reaction to possibly occur. If the collision orientation is incorrect, the particles simply bounce off each other, and no reaction occurs.



Unfavourable orientation.
Reaction is unlikely.

Favourable orientation.
Reaction is likely.

$$2HI(g) \rightarrow H_2(g) + I_2(g)$$

FIGURE 15.3.5 A reaction between colliding molecules is more likely to occur if the orientation of the collision is favourable.

FACTORS INCREASING COLLISION FREQUENCY AND COLLISION ENERGY

In Module 15.1, you saw that the rate of a reaction can be changed by factors such as the surface area, concentration, pressure of reactants and also the reaction conditions such as temperature and presence of a catalyst.

In this section we will explain these effects in relation to collision theory. Table 15.3.1 summarises how each factor is related to an increase in the proportion of successful collisions and a subsequent increase in reaction rate. This can be due to an increase in the frequency or energy of collisions, or due to the lowering of the required activation energy. For temperature, more than one of these effects occurs.

TABLE 15.3.1 Factors that increase reaction rate

Factor	Effect on reactant molecules
concentration	increase in frequency of collisions
pressure	increase in frequency of collisions
surface area	increase in frequency of collisions
temperature	increase in frequency and energy of collisions
presence of a catalyst	increase in proportion of molecules with sufficient energy

Changing concentration or pressure

In Module 15.1, you learnt that the rate of a reaction can be increased by increasing the concentration of a reacting solution or increasing the pressure of a reacting gas. This can be explained by collision theory.

The rate of a reaction increases when the frequency of collisions between reactants increases. When the concentration of a solution increases, there are more reactant particles moving randomly in a given volume of solution (Figure 15.3.6). The frequency of collisions consequently increases and so more successful collisions occur in a given time.

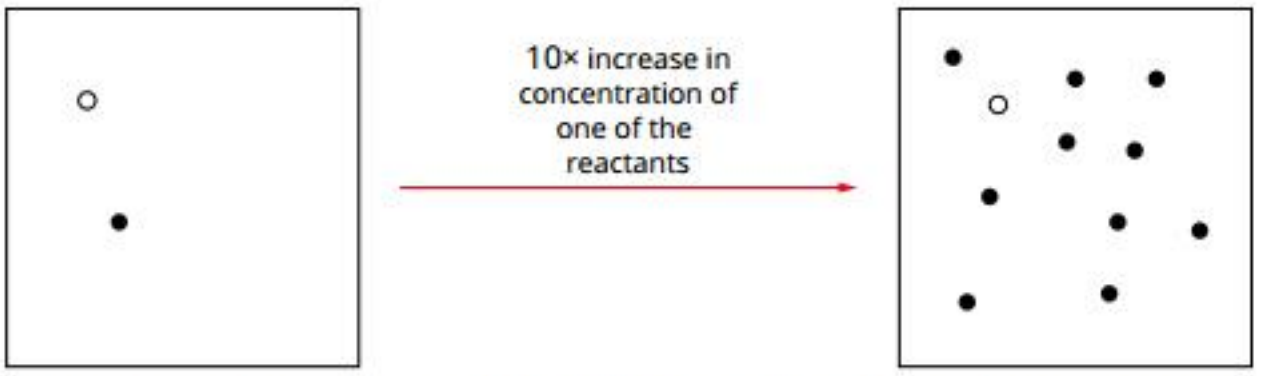


FIGURE 15.3.6 On the left, the concentration of both reactants is low. On the right, the concentration of one of the reactants (black dots) has been increased 10-fold, resulting in an increase in collision frequency.

For a reaction in the gas state, the pressure of the gases can be increased either by adding more gas to a fixed volume container or by decreasing the volume of a container with a variable volume, such as a gas syringe. Increasing the pressure increases the concentration of gas molecules, causing more frequent collisions and increasing the number of successful collisions in a given time.

When using collision theory to explain the effect of concentration, pressure and surface area on the rate of a chemical reaction, you must discuss the effect on either collision frequency or the number of successful collisions per unit of time.

Changing surface area

When a solid is involved in a reaction, only the particles at the surface of the solid are involved in the reaction. The number of particles at the surface depends on the surface area of the substance. As you can see in Figure 15.3.7, breaking a certain amount of solid into smaller parts means that more particles are present at the surface and available to react. The surface area has increased.

As a consequence of the greater number of exposed particles, the frequency of collisions between these particles and the other reactant particles increases, and so the reaction occurs more rapidly.

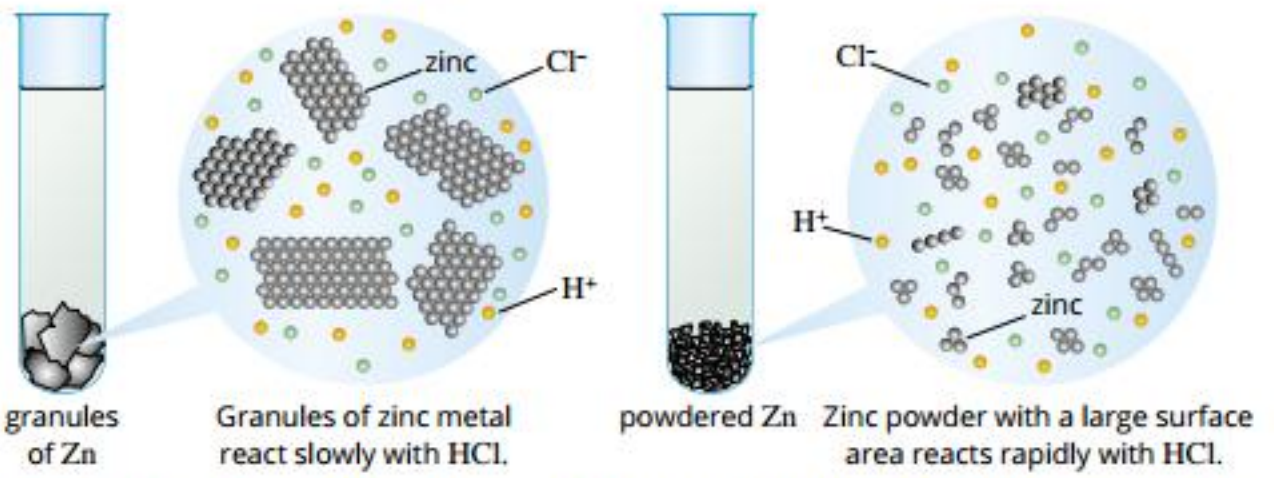


FIGURE 15.3.7 The reaction of hydrochloric acid and zinc. As the surface area of zinc increases, the rate of reaction with hydrochloric acid increases. (The H_3O^+ ion is represented as H^+ in the diagrams.)

The effect of increasing surface area can be seen when setting up an open fire at home or on a camp. It is best to first light a pile of kindling rather than trying to directly light large logs. The kindling has a larger surface area than the logs, so it catches fire more easily and will then burn rapidly, providing enough sustained heat energy to make the logs catch fire as well.

Worked example 15.3.1

USING COLLISION THEORY TO EXPLAIN CHANGES IN RATES OF REACTIONS

There have been many explosions in underground coal mines due to the presence of coal dust in air. Explain this observation in terms of collision theory.	
Thinking	**Working**
Consider the state of the reactants.	Coal is a solid. In the mine, there would be lumps of coal and also powdered coal present as coal dust in air.
Relate the state of the reactant to the factor that affects the reaction rate (surface area) and explain in terms of collision theory.	The surface area of powdered coal is greater than that of solid coal. When the surface area increases, the frequency of collisions increases and so the rate of reaction increases.
Return to the question to complete your answer. Reaction rate is faster for greater surface area of reactant (coal).	An explosion is a very fast reaction. The very large surface area of the coal dust allows for an increase in the frequency of collisions with reacting particles, which increases the reaction rate so much that explosions occur.

➤ Try yourself 15.3.1

USING COLLISION THEORY TO EXPLAIN CHANGES IN RATES OF REACTIONS

Iron anchors recovered from shipwrecks at considerable depths can show little corrosion (oxidation) after years in the sea, whereas anchors recovered from shallow water are badly oxidised and corroded. Use collision theory to provide a possible reason for this observation.

Reaction temperature and Maxwell–Boltzmann distribution

As you have seen, a reaction can be made to occur more rapidly by increasing the concentration of the reactants or, for solids, increasing the surface area. A change in temperature can also have a major effect on the rate of a reaction. This effect is via a change to the **kinetic energy** of particles of the reactants.

At any particular temperature, the particles in a substance have a range of kinetic energies. Although most of the particles have similar kinetic energies, there are always some particles with a high energy or a low energy. This range of energies is shown on a graph called a **Maxwell–Boltzmann distribution curve** (Figure 15.3.8), also known as a **kinetic energy distribution diagram**. The peak of the graph shows the energy of the greatest number of particles and the area under any given portion of the graph represents the number of particles with that particular range of energies.

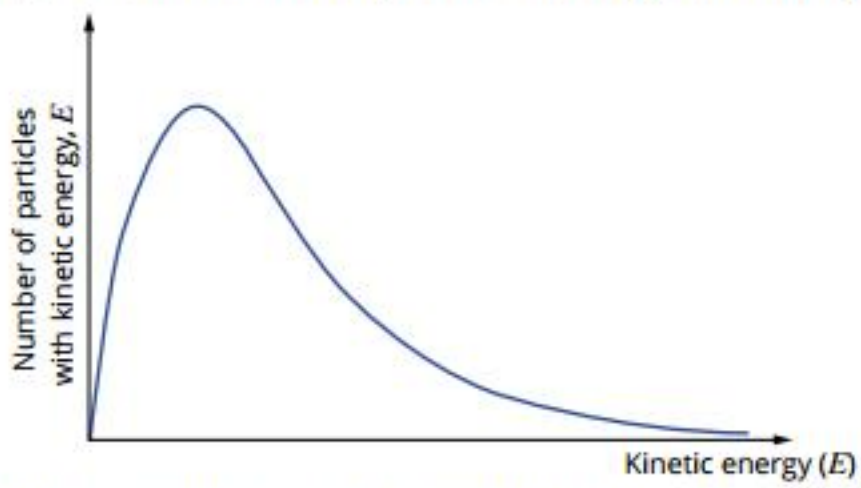


FIGURE 15.3.8 This Maxwell–Boltzmann curve shows the distribution of energies of particles in a sample at a particular temperature.

The activation energy for a reaction involving the particles displayed in the Maxwell–Boltzmann plot can be plotted on the *x*-axis of the graph (Figure 15.3.9). During a reaction at a given temperature, if only a proportion of the reactant particles have kinetic energy that is equal to or greater than the activation energy, only this proportion will react. You can see this in Figure 15.3.9 as a small, shaded area to the right of the activation energy, E_a.

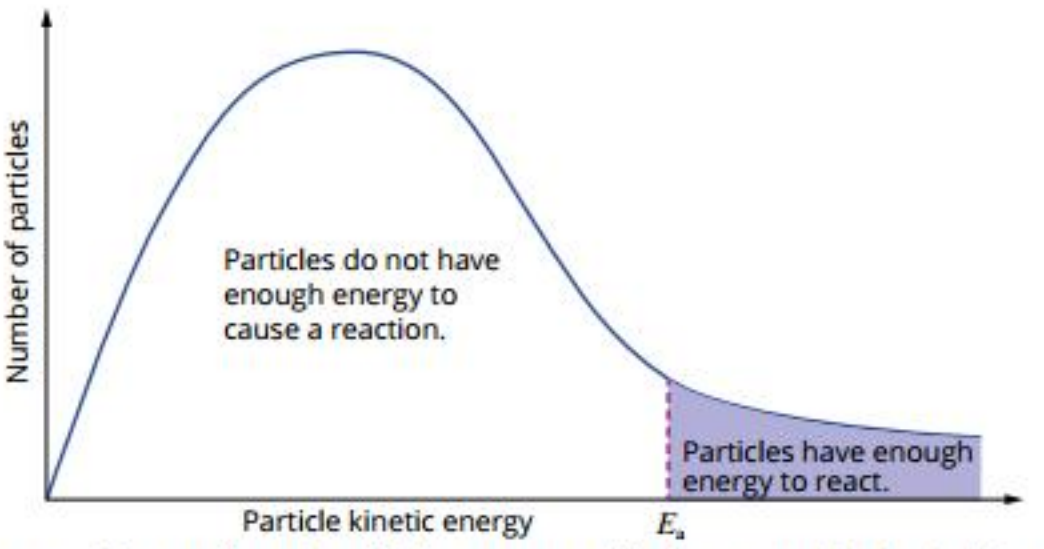

Number of particles
Particles do not have enough energy to cause a reaction.
Particles have enough energy to react.
Particle kinetic energy
E_a

FIGURE 15.3.9 Only a small number of higher energy particles (represented by the shaded area) have sufficient energy to overcome the activation energy barrier.

The relationship between kinetic energy and velocity is given by the formula $KE = \frac{1}{2}mv^2$. As the temperature of a reaction system increases, the average kinetic energy of the particles increases and the average speed of the particles in the system increases as well. This is illustrated in Figure 15.3.10, in which the range of kinetic energies for a gas at three different temperatures is shown. Note that the area under the curve, which is equal to the total number of particles in the sample, stays constant when the temperature is changed. As the temperature increases, the increasing average kinetic energy of the particles can be seen by the movement to the right of the peak in the Maxwell–Boltzmann curve.

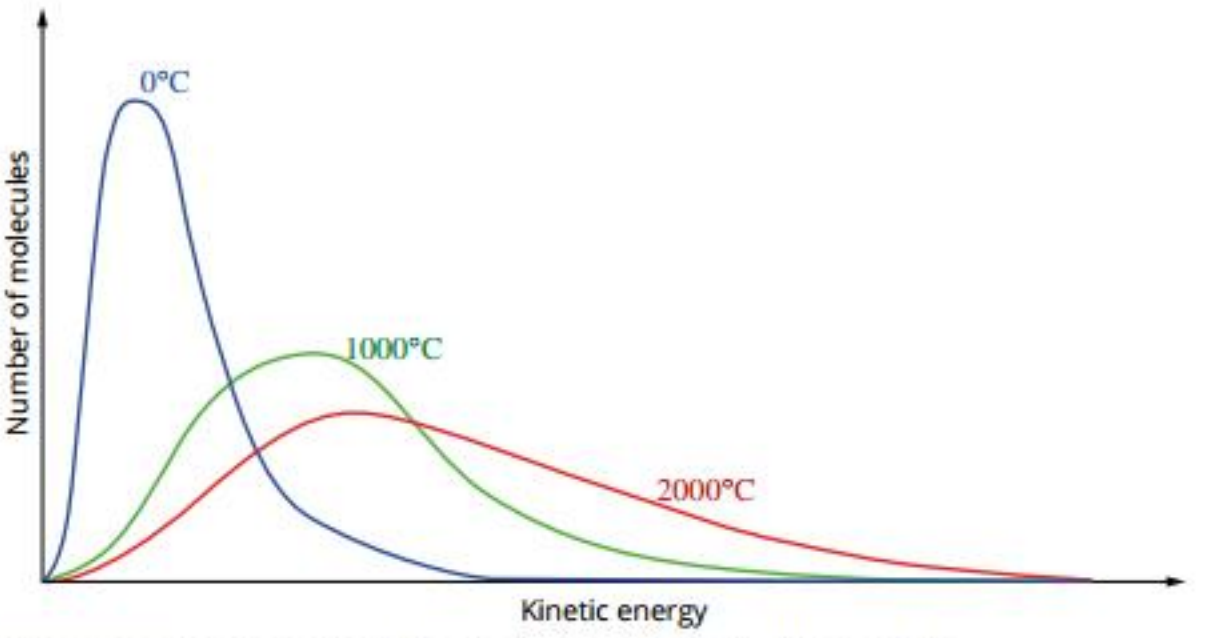


FIGURE 15.3.10 Kinetic energy distribution for a gas at a range of temperatures.

i The effect of increasing temperature on the rate of reaction is mainly through increasing kinetic energy of most particles resulting in more collisions and a greater proportion of reacting particles that have energies equal to or greater than the activation energy for the reaction. These two factors increase the proportion of successful collisions.

As the temperature of a reaction increases, the increased speed of particles causes more frequent collisions, increasing the frequency of successful collisions and the rate of reaction.

The increased kinetic energy of the particles also means that collisions occurring at higher temperatures have greater energy than those at lower temperatures. More particles will have energies that are greater than or equal to the activation energy and so the proportion of successful collisions also increases.

When the temperature increases, the increase in reaction rate due to the increased energy of the collisions significantly outweighs the increase in reaction rate due to the increased frequency of collisions. A temperature increase of just 10°C causes the rate of many reactions to double (an increase of 100%), but it can be shown that this is not due to the increased frequency of collisions. The frequency of collisions only increases by about 3% when the temperature increases by 10°C. The main reason why the reaction rate increases is that more particles have sufficient energy to overcome the activation energy barrier of the reaction.

15.3 Review

SUMMARY

- Collision theory is a theoretical model that accounts for the rates of chemical reactions in terms of collisions between particles during a chemical reaction.
- According to collision theory, for a reaction to occur, the reactant particles must:
  - collide with each other
  - collide with sufficient energy to break the bonds within the reactants
  - collide with the correct orientation to break the bonds within the reactants and so allow the formation of new products.
- The activation energy of a reaction is the minimum amount of energy required to break reactant bonds to allow a reaction to proceed. It is the minimum amount of energy that a collision between reactant particles must possess for a reaction to occur.
- An energy profile diagram (Figure 15.3.11) shows the activation energy as a peak of highest potential energy between the energy of the reactants and the energy of the products. It also shows the change in enthalpy (ΔH) during the reaction.

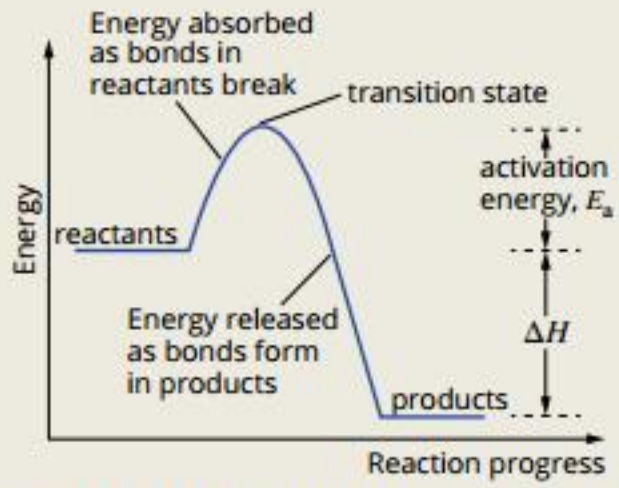


FIGURE 15.3.11 An energy profile diagram, showing activation energy and change in enthalpy.

- Collision theory can be used to explain the increase in rate of reaction by an increase in:
  - concentration of a reactant solution
  - pressure of a gaseous reactant
  - surface area of a solid reactant
  - temperature.
- Increase in concentration, pressure or surface area results in an increase in the:
  - frequency of collisions between reactants
  - number of successful collisions in a given time.
- Increase in temperature results in an increase in the:
  - frequency of collisions between reactants and the number of successful collisions in a given time
  - (most importantly), energy of collisions, so an increased proportion of collisions has an energy larger than the activation energy for the reaction.
- A Maxwell–Boltzmann plot indicates the kinetic energy distribution of all particles in a substance. It often includes a value for E_a annotated on the *x*-axis. Particles in the group to the right of this value have sufficient kinetic energy to react.

15.3 Review *continued*

KEY QUESTIONS

Describe

1 Most collisions between reacting particles are not successful in terms of forming products. Name the other factors that are required for successful collisions between reactants.

2 Define the activation energy of a chemical reaction.

3 Identify the appropriate term for the following statements.

- **a** In an exothermic reaction, the energy of the products is *higher/lower* than the energy of the reactants.
- **b** In an endothermic reaction, the energy of the products is *higher/lower* than the energy of the reactants.

4 Identify the physical characteristic that is measured and displayed in a Maxwell–Boltzmann plot.

5 True or false? The stage of a reaction where bonds are broken in the reactants is exothermic.

Apply

6 The reaction between magnesium (Mg(s)) and hydrochloric acid (HCl(aq)) can be represented by the following chemical equation:

$$Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$$

Use collision theory to explain why this reaction is faster with 1.0 M HCl compared to 0.1 M HCl.

7 Choose the correct term in each sentence to explain why a chemical reaction may occur very slowly.

- **a** The activation energy may be *very large/very small*.
- **b** The temperature may be *high/low*.
- **c** The frequency of collisions may be *too low/too high*.

8 The temperature of a reaction mixture is increased.

- **a** Describe the effect on the number of reacting particles in the reaction mixture.
- **b** Describe the change to the Maxwell–Boltzmann plot of the particles in the reaction mixture.

Analyse

9 Apply your knowledge of the collision model of particle behaviour to explain the following observations:

- **a** Surfboard manufacturers find that fibreglass plastics set within hours in summer but may remain tacky for days in winter.
- **b** A bottle of fine aluminium powder has a sticker warning 'Highly flammable, dust explosion possible'.
- **c** A potato cooks much more slowly in a pot of boiling water on a trekking holiday in Nepal than a potato boiled in a similar way in the Australian bush.

10 When 1 mole of methane gas burns completely in oxygen, the process of bond breaking uses 3380 kJ of energy and 4270 kJ of energy is released as new bonds form.

- **a** Write a balanced chemical equation for the reaction.
- **b** Calculate the value of the heat of reaction, ΔH, for the reaction.
- **c** Draw and label an enthalpy diagram to determine the changes in energy during the course of the reaction.

11 The formation of hydrogen iodide from its elements is represented by the equation:

$$H_2(g) + I_2(g) \rightarrow 2HI(g)$$

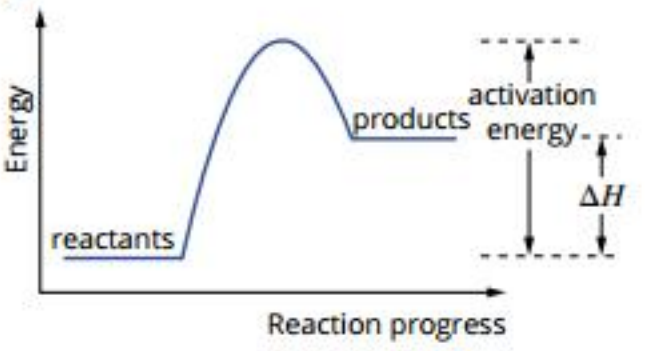
This reaction has an activation energy of $+167\,kJ\,mol^{-1}$ and the heat of reaction, ΔH, is $-9\,kJ\,mol^{-1}$. Determine the activation energy for the reverse reaction, the decomposition of 2 moles of hydrogen iodide.

12 A number of experiments involving the reaction between 100 mL of 1M hydrochloric acid and 5 g of calcium carbonate were carried out. Sort experiments A–D and place them in increasing order of rate of reaction (slowest to fastest).

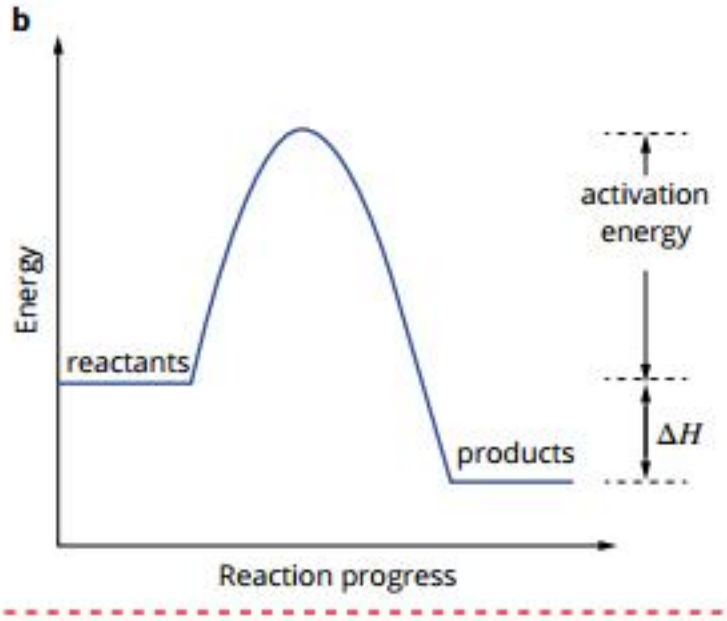
- **A** Powdered $CaCO_3$ and 40°C reaction temperature
- **B** $CaCO_3$ pieces and 15°C reaction temperature
- **C** Powdered $CaCO_3$ and 15°C reaction temperature
- **D** Powdered $CaCO_3$ and 25°C reaction temperature

13 Compare the energy change for the following two reactions, a and b.

a



b



15.4 Catalysts

BY THE END OF THIS MODULE, YOU SHOULD BE ABLE TO:

- explain that a catalyst increases the rate of chemical reaction by providing an alternative reaction pathway with a lower activation energy compared to the uncatalysed reaction
- recall that catalysts are not consumed in chemical reactions
- construct and analyse energy profile diagrams for catalysed and uncatalysed reactions
- use activation energy annotations on a Maxwell–Boltzmann plot to analyse the effect of a catalyst on number of reacting particles
- differentiate between a homogeneous catalyst and heterogeneous catalyst
- recall that two key catalyst types are (i) metals and metal compounds (inorganic catalysts) and (ii) enzymes (organic catalysts).

In this module, you will learn how various types of **catalysts** increase the rate of reaction. The change in reaction rate when a catalyst is present is often very substantial. The action of a catalyst affects energy changes during the reaction and can be understood using collision theory. Catalysts play an important role in industrial chemistry, in limiting air pollution, in controlling biochemical processes, and in the efficient production of many chemicals such as ammonia, sulfuric acid and ethanol.

CATALYSTS AND ACTIVATION ENERGY

You have already learnt that the potential energy changes associated with a reaction can be represented as an energy profile diagram of the reaction over time. An energy profile diagram for an exothermic reaction is shown in Figure 15.4.1.

As described in Module 15.3, the activation energy is the minimum amount of energy required for a reaction to take place. On the energy profile diagram, the activation energy is measured from the energy of the reactants to the peak of the energy profile diagram. The enthalpy change, ΔH, can also be represented on an energy profile diagram and is equal to the difference in energy between the products and the reactants.

Some reactions occur very readily because they have very small activation energies, E_a. These reactions need only a small amount of energy to be absorbed for bonds in the reactants to be broken. Many reactions occur much more rapidly in the presence of a particular element or compound known as a catalyst. Catalysts are not consumed during the reactions they speed up, and so do not appear as either reactants or products in chemical equations. Catalysts are able to cause a reaction to occur more quickly because they provide a new **reaction pathway**, which results in a dramatically reduced activation energy barrier for the overall reaction, as seen in the energy profile diagram in Figure 15.4.2 on page 440.

With the catalyst lowering the activation energy, colliding particles are more likely to have energies that exceed this lower barrier, causing the bonds in the reactants to be broken more frequently. As a result, a greater proportion of collisions are successful, that is, they lead to the formation of products. Thus, the reaction rate is increased.

The catalysed reaction has the same overall energy change (ΔH) and the same amount of product(s) is formed—the catalysed reaction goes faster not further.

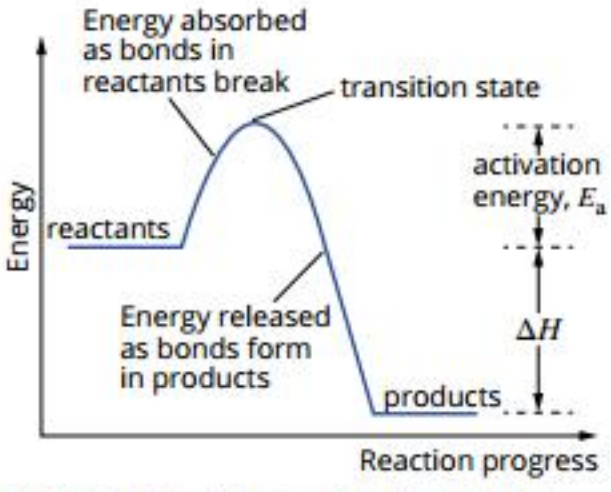


FIGURE 15.4.1 Energy profile diagram of an exothermic reaction such as burning natural gas.

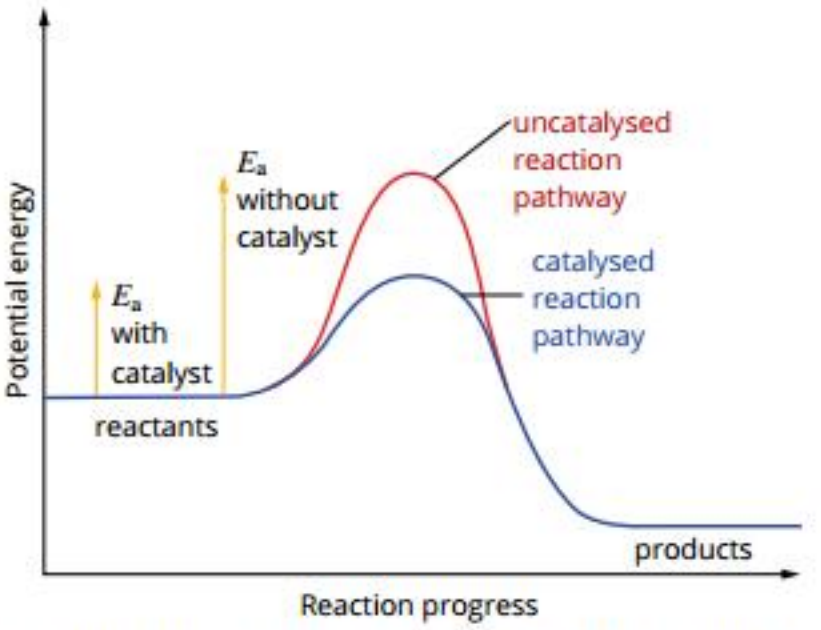


FIGURE 15.4.2 Energy profile diagrams of a catalysed and uncatalysed reaction.

Catalysts and Maxwell–Boltzmann plots

In Module 15.3, you learnt that a Maxwell–Boltzmann curve shows the distribution of kinetic energies of particles in a sample at a particular temperature. It reflects the fact that the particles of a substance have a range of energies and that, at a particular temperature, some of these particles have energies that are sufficient to initiate a chemical reaction while particles with lower kinetic energies will not react. The energy required for a successful collision is often plotted on the x-axis as E_a, activation energy.

The Maxwell–Boltzmann curve in Figure 15.4.3 shows the smaller number of particles with energies that exceed the activation energy in an uncatalysed reaction (shaded in red) compared with the number of particles with energies that exceed the activation energy in a catalysed reaction (sum of the regions shaded in red and blue). When the catalyst provides an alternate reaction pathway, the energy required for the reaction decreases and, as shown in Figure 15.4.3, E_a moves to the left. In the presence of a catalyst, a greater number of particles will react, resulting in an increased reaction rate.

Catalysts only lower the activation energy for a reaction. There is no change to ΔH for the reaction.

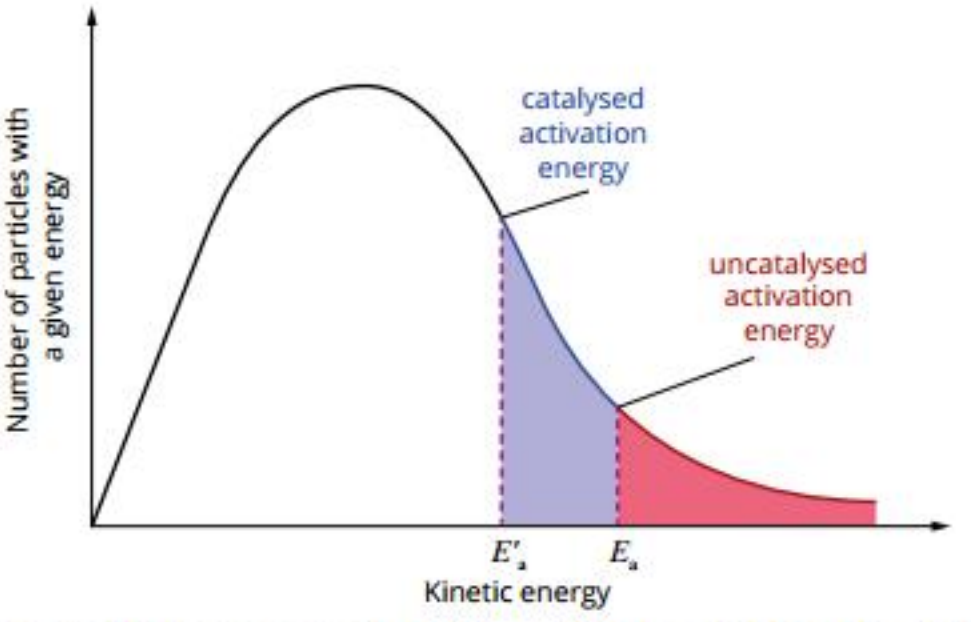


FIGURE 15.4.3 A catalyst provides a reaction pathway with a lower activation energy, increasing the proportion of particles whose energy exceeds the activation energy and will therefore react.

TYPES OF CATALYSTS

Depending on the physical state of reactants and the catalyst, catalysts can be divided into two groups.

- **Homogeneous catalysts** are in the same physical state as the reactants of the reaction. Usually, both catalyst and reactants are dissolved in solution or combined as a gaseous mixture. An example of this type of catalyst is enzymes (described below), which are usually soluble in an aqueous solution. They exist in the same state as the dissolved reactants of the reaction. Homogeneous **catalysis** occurs in the upper atmosphere and has contributed to the depletion of the ozone layer. Chlorine atoms in the gaseous state act as catalysts in the decomposition of ozone gas into oxygen gas. The chlorine atoms may have come from chlorofluorocarbons (CFCs) released into the atmosphere from refrigerators or air conditioners.
- **Heterogeneous catalysts** are in a different physical state from the reactants of the reaction. This generally occurs when small particles of solid catalyst are combined with liquid, aqueous or gaseous reactant mixtures. Many of these catalysts are transition metals. You may be familiar with the catalysed decomposition of a hydrogen peroxide solution using the black powder manganese (IV) oxide ($Mn(IV)O_2$) where bubbles of hydrogen and oxygen gas are produced. This is an example of the use of a heterogeneous catalyst. A powdered or sponge-like form of a solid catalyst is often used to provide the greatest possible surface area. With a larger surface area, more reactant molecules can be adsorbed on the catalyst surface allowing the reaction to proceed even faster.

The chemical industry uses catalysts extensively. Chemists prefer to use heterogeneous catalysts for industrial processes because they are:

- more easily separated from the products of a reaction and therefore easier to reuse
- effective in a wide range of reactions and processes
- able to be used at high temperatures.

Heterogenous catalyst solids act by **adsorption**. Reactant molecules are attracted to their surface in an association which distorts their covalent bonds and may even break them completely. This allows a reaction to proceed more easily than it would if the solid were absent. Transition metals tend to be good catalysts with partially filled d-orbitals, easily accepting or donating electrons to allow the formation of transient bonds with reactants. These transient bonds can weaken bonds in adsorbed reactant, facilitating rearrangement of atoms to form new products. Common examples of these metals are nickel, palladium, iron and platinum. These solid surfaces provide a new reaction pathway for the reaction to occur—one that has a significantly lower activation energy.

Figure 15.4.4 shows metal cations on a silica-alumina zeolite surface adsorbing gas molecules. Layers of porous zeolite are used in petroleum refineries during the **catalytic cracking** process. Larger hydrocarbon molecules are broken down into smaller more useful molecules.

Catalysts lower the activation energy by providing an alternative reaction pathway for the reaction. This increases the proportion of reactant particles with energies equal to or greater than the lower activation energy. This increases the proportion of successful collisions.

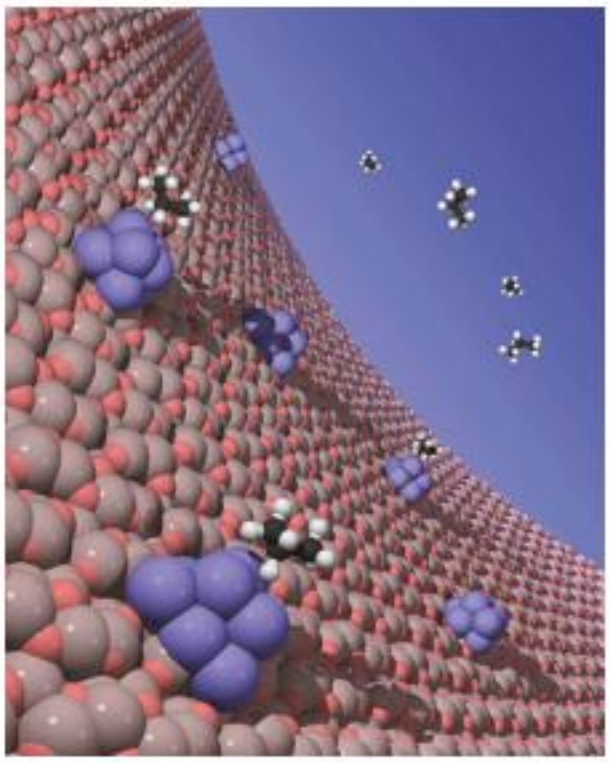


FIGURE 15.4.4 A representation of the structure of a synthetic zeolite catalyst showing hydrocarbon reactants adhering to metal cations (blue) on the zeolite surface (brown).

Heterogeneous catalysis and the Haber process

The **Haber process** is an important commercial reaction that produces ammonia gas, which is used to make fertilisers, nylon, explosives and some pharmaceuticals. In the Haber process, hydrogen and nitrogen gas are converted to ammonia (NH_3), using a catalyst such as powdered iron.

The reaction is represented by the equation:

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \quad \Delta H = -91\,\text{kJ mol}^{-1}$$

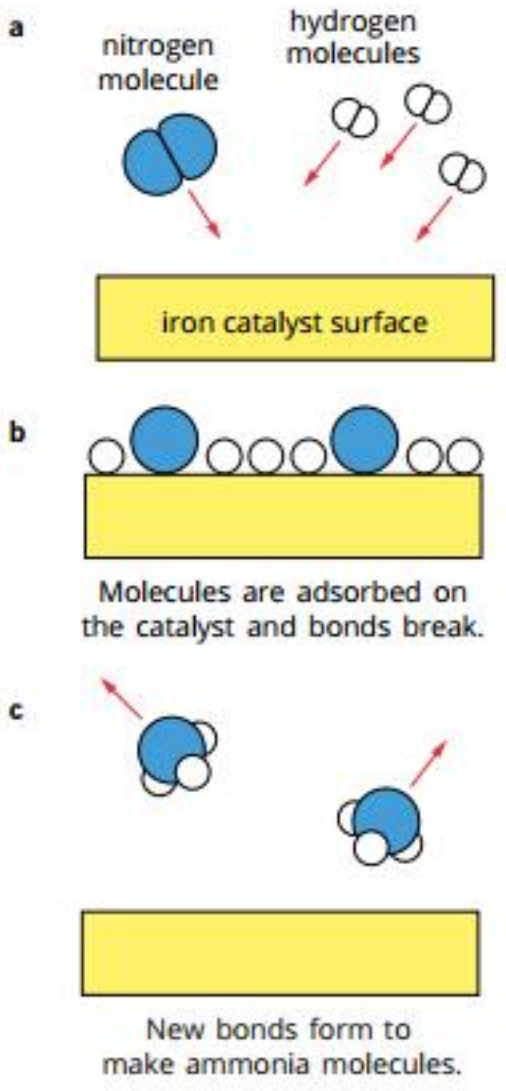


FIGURE 15.4.5 Behaviour of a catalyst in ammonia production (Haber process). (a) Nitrogen and hydrogen molecules approach the iron catalyst surface. (b) The nitrogen and hydrogen molecules adsorb on the surface of the catalyst and their covalent bonds are broken. (c) The hydrogen and nitrogen atoms readily combine to form ammonia molecules. The molecules then leave the catalyst surface, and the catalyst remains unaltered by the reaction.

Hydrogen and nitrogen molecules both adsorb onto the iron surface (Figure 15.4.5a). As they attach themselves to the surface, the covalent bonds within their molecules break (Figure 15.4.5b). The hydrogen and nitrogen atoms now readily combine to form ammonia molecules and move away (desorb) from the iron surface (Figure 15.4.5c). The catalyst remains unaltered by the reaction. Without a catalyst, temperatures over 3000°C are needed for the reaction to occur. The catalyst allows the manufacture of ammonia to proceed at an economical rate using a temperature of about 500°C.

The iron catalyst provides an alternative reaction pathway that dramatically reduces the activation energy barrier—the energy needed to break the covalent bonds in the nitrogen and hydrogen molecules. Even though collisions are less frequent at 500°C than at 3000°C, a greater proportion of colliding particles have sufficient energy to successfully react. The yield of the Haber process is further described in the Chemical Synthesis section of Unit 4 Topic 2.

Heterogeneous catalysis of combustion products

Catalysts in the exhaust pipe of cars convert carbon monoxide and nitrogen oxide, formed in the engine, to the non-toxic gases carbon dioxide and nitrogen. In this way, air pollution from exhaust gases is reduced.

$$2NO(g) \rightarrow N_2(g) + O_2(g)$$
$$2CO(g) + O_2(g) \rightarrow 2CO_2(g)$$

Unburnt hydrocarbons are also converted by the catalyst to carbon dioxide and water.

$$2C_8H_{18}(g) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(g)$$

The catalyst is usually a mixture of platinum, palladium and rhodium metals and aluminium oxide, and it is mounted on a honeycomb-shaped support (Figure 15.4.6). Millions of tiny pores in the metals provide a large surface area.

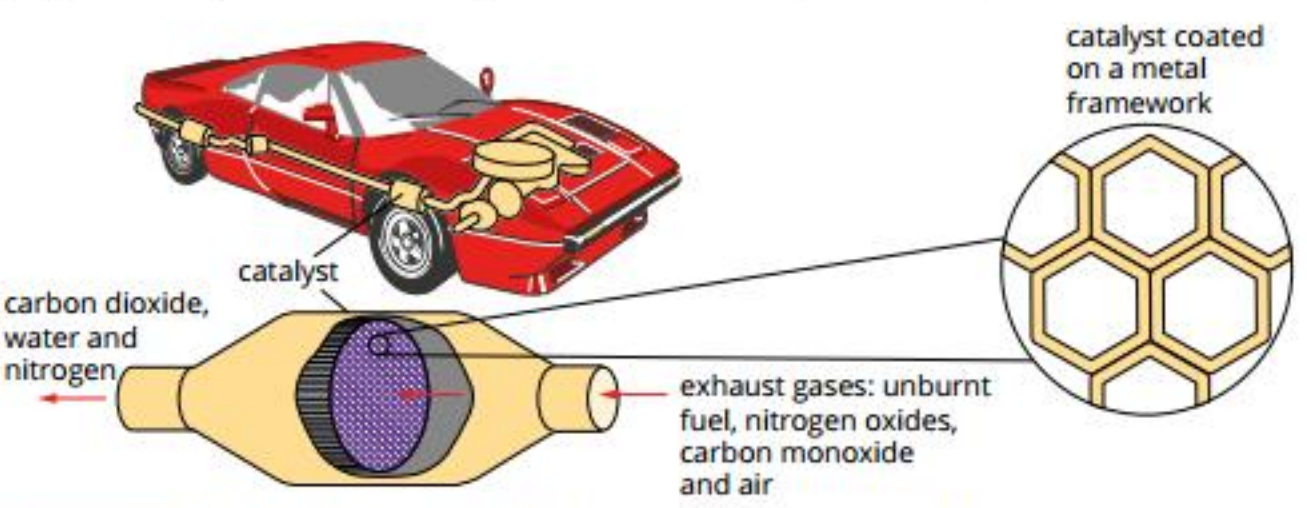

catalyst coated on a metal framework
catalyst
carbon dioxide, water and nitrogen
exhaust gases: unburnt fuel, nitrogen oxides, carbon monoxide and air

FIGURE 15.4.6 A catalyst fitted in the exhaust system of a car reduces air pollution.

Enzymes as catalysts

The catalysts described so far are **inorganic**—they are not of biological origin. **Enzymes** are **organic** catalysts. They are large biological molecules, the smallest containing about 1000 atoms, which are typically proteins but may also be RNA molecules. Enzymes catalyse a wide range of processes (over 5000) in living organisms and are found almost everywhere in our bodies assisting in everything from digesting our food to copying our DNA. They are essential for biochemical reactions in our cells.

Like inorganic catalysts, enzymes are not consumed in chemical reactions, and they increase reaction rates by lowering the activation energy of chemical reactions. Enzyme catalysis can involve both homogeneous catalysis, where the enzyme and its reacting molecules are freely soluble in solution, or heterogeneous catalysis where the enzyme molecule is embedded into a solid structure (such as a cell wall) with the reactant molecules residing in the intra- or extra-cellular fluid.

A major difference between enzymes and other types of catalysts is their specificity. Enzymes tend to act on specific molecules (**substrates**) and therefore will often catalyse a single chemical reaction or a small number of closely related reactions. This is due to the particular 3-dimensional shape of the substrate-binding site (Figure 15.4.7). Each enzyme will have an optimum range of temperature and pH. Outside of this range, chemical changes (unfolding) of the protein structure compromise the all-important binding site and consequently, a loss of catalytic activity occurs. As the optimum pH and temperature ranges for enzyme activity are generally similar to that of living organisms, enzymes are viewed as 'green' alternatives for reactions that would otherwise use high temperatures, pressures and/or involve toxic chemicals.

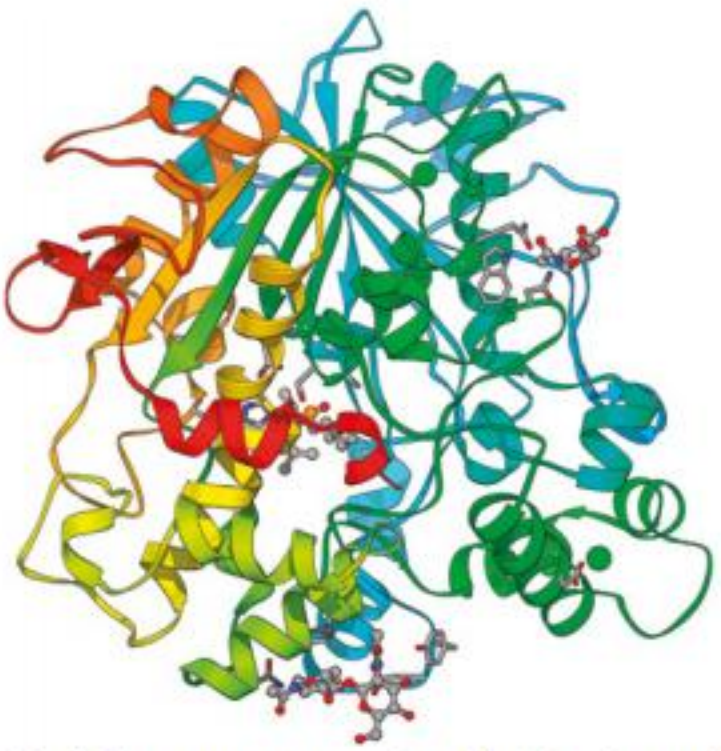


FIGURE 15.4.7 A model of a lipase enzyme, an organic catalyst, showing complex folding of its protein chain and several molecules attached to its binding sites. Lipase is a catalyst that breaks down fats in the digestive system of the human body.

15.4 Review

SUMMARY

- The rate of a reaction can be increased by using a catalyst, which itself, is not used up in the reaction.
- A catalyst provides an alternative reaction pathway that has a lower activation energy, E_a.
- Energy profile diagrams (Figure 15.4.8), which can include catalysed and uncatalysed pathways, may be used to represent the enthalpy changes and activation energy associated with a chemical reaction. For a catalysed reaction, E_a is less but ΔH is unchanged.

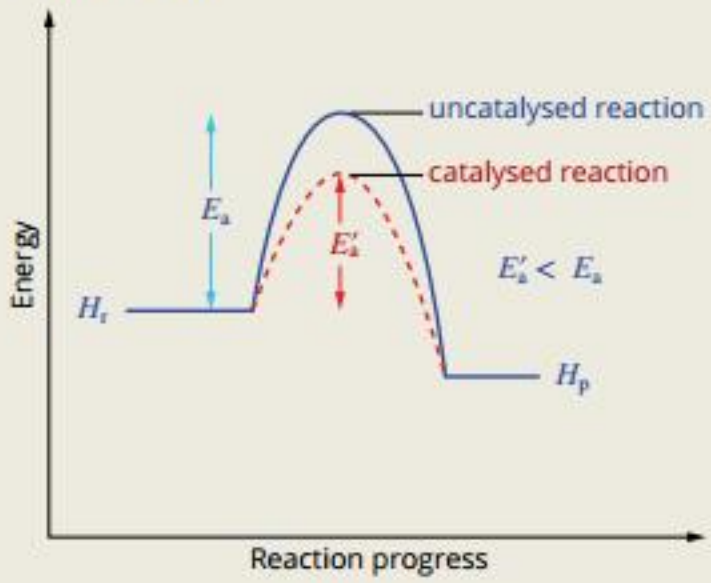


FIGURE 15.4.8 Energy profile diagram of a reaction showing the effect of a catalyst.

- When a catalyst is present, a greater proportion of the collisions between particles exceed the activation energy barrier of the reaction and therefore leads to a faster reaction rate. This is diagrammatically represented on the Maxwell–Boltzmann plot as a shift to the left in the value of E_a (x-axis).
- Catalysts can be homogeneous or heterogeneous. An important example of a heterogeneous catalyst is the use of iron to catalyse the Haber process.
- Catalysts can be inorganic (such as transition metals) or organic (such as enzymes).
- Enzymes are macromolecules that react with a specific substrate—different enzymes catalyse a wide range of biochemical reactions in living organisms. They function at mild conditions and are sensitive to pH and temperature.

KEY QUESTIONS

Describe

1 Define the term 'catalyst'.

2 State what an enzyme is.

3 Contrast organic and inorganic catalysts.

Apply

4 A scientist uses platinum metal particles to increase the rate of production of sulfur trioxide:

$$2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$$

Identify if this example uses a homogeneous catalyst or heterogeneous catalyst.

5 In terms of the energy of colliding reactant particles, explain how a catalyst increases the rate of a chemical reaction.

6 **a** Explain why surface properties are important to the operation of heterogeneous catalysts.

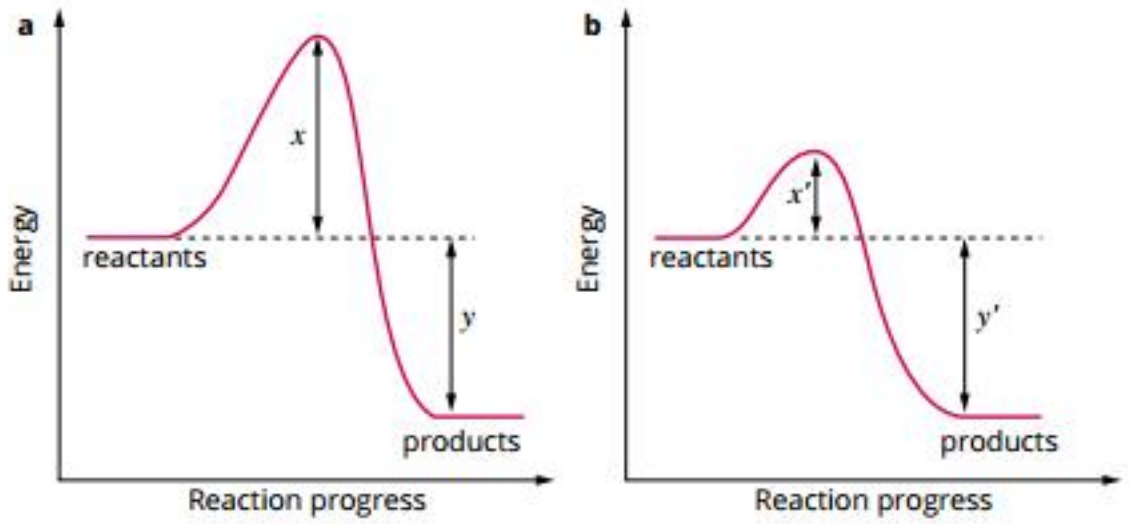
b Many industrial catalysts are made into porous pellets. Suggest a reason for this.

7 The energy of a reaction mixture is determined over time for a reaction with and without a catalyst.

a Identify the reaction characteristics which are labelled x, x', y, y'.

b Describe which reaction a or b is the catalysed reaction.

c Describe the overall energy change during the reaction and explain any effect of the catalyst on this quantity.



8 The axes of a Maxwell–Boltzmann plot indicate the kinetic energy of particles and the number of particles.

a Identify which of these is on the *x*-axis and which is on the *y*-axis.

b Describe the shift of the E_a value (left or right) when a catalysed reaction is performed at the same temperature but without the catalyst present.

Analyse

9 Using the example provided in Question 7 explain the difference in the reaction rate between the two reactions.

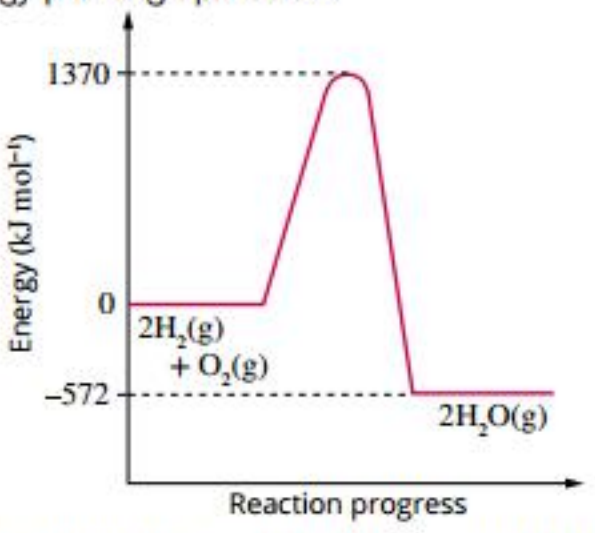
10 The rate of a chemical reaction can be increased by increasing temperature and/or by adding a catalyst. With reference to collision theory, contrast these two approaches to increasing reaction rates.

11 If a sugar cube is held in the flame of a candle, the sugar melts and browns but does not burn. However, the cube burns if salt is first rubbed into it, even though the salt does not react. Determine the effect of the salt on the activation energy of this combustion reaction.

12 Many major car makers have plans for hydrogen-powered cars. In the fuel cells of these cars, hydrogen reacts with oxygen from the air to produce water.

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$

Energy changes for the reaction are shown in the energy profile graph below.



a Determine the magnitude of the activation energy of this reaction.

b Determine ΔH for this reaction.

Several groups of scientists have claimed to have split water into hydrogen and oxygen using a molybdenum catalyst:

$$2H_2O(g) \xrightarrow{Mo} 2H_2(g) + O_2(g)$$

c Sketch energy change graphs for this reaction with and without the presence of a catalyst.

d Determine the value of ΔH for this water-splitting equation.

Chapter review

15

KEY TERMS

acid rain
activation energy
adsorption
average rate of reaction
catalysis
catalyst
catalytic cracking
chemical reaction
collision theory
concentration
concentration–time curve
endothermic
energy profile diagram
enzyme
exothermic
Haber process
heterogeneous catalyst
homogeneous catalyst
initial rate of reaction
inorganic
instantaneous rate of reaction
kinetic energy
kinetic energy distribution diagram
Maxwell–Boltzmann distribution curve
organic
potential energy
pressure
rate of reaction
reactant
reaction pathway
substrate
surface area
transition state

KEY QUESTIONS

Describe

1 Identify which one of the following is the correct definition of rate of reaction.
- **A** the time it takes for all of a reactant to be used up
- **B** how fast a reaction is going at the end of 1 minute
- **C** how much a reaction is bubbling
- **D** the change in concentration of reactants or products over time

2 Identify which of the following is the correct unit for measuring the rate of a reaction (choose all that apply).
- **A** $mol^{-1} L s^{-1}$
- **B** $mol L^{-1} s^{-1}$
- **C** $M^{-1} s$
- **D** $M s^{-1}$

3 Identify which of the following changes would decrease the rate of the reaction between zinc metal and dilute hydrochloric acid.
- **A** increasing the temperature of the hydrochloric acid
- **B** decreasing the size of the pieces of zinc
- **C** decreasing the concentration of the hydrochloric acid
- **D** decreasing the temperature of the hydrochloric acid

4 According to collision theory, select which one of the following is *not* essential for a reaction to occur.
- **A** Molecules must collide to react.
- **B** The reactant particles should collide with the correct orientation.
- **C** The reactant particles should collide with enough energy to overcome the activation energy barrier.
- **D** The reactant particles should collide with double the energy of the activation energy.

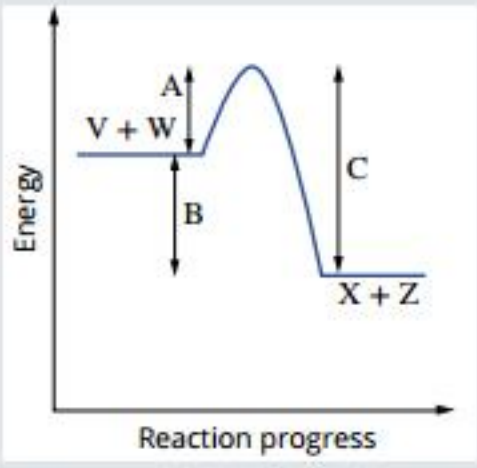
5 According to collision theory, state what must happen for a reaction to occur.

Apply

6 Consider the reaction between solutions V and W that produces X and Z according to the equation:

$$V(aq) + W(aq) \rightarrow X(aq) + Z(aq)$$

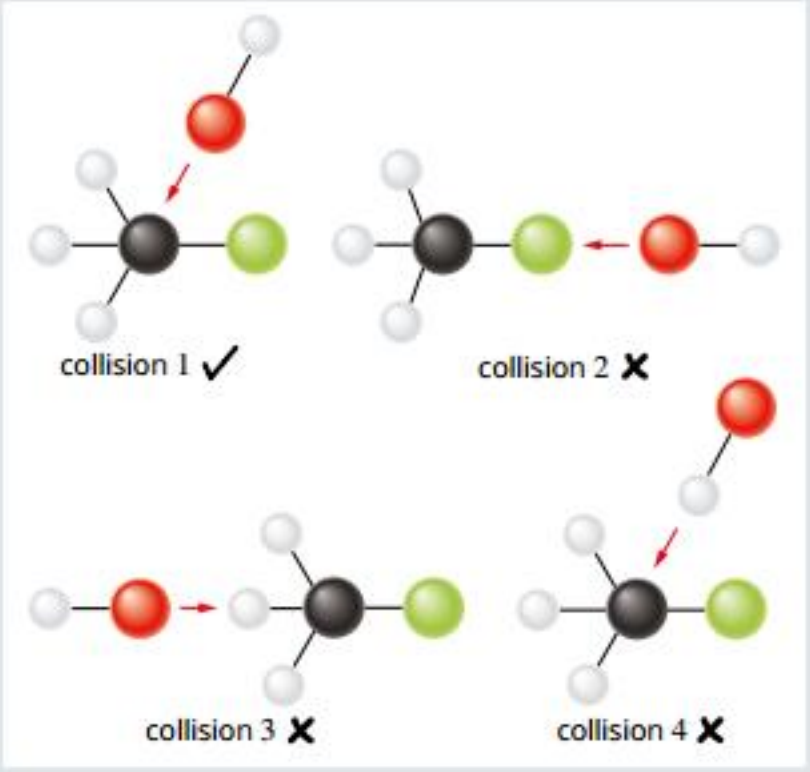
The energy profile diagram for this process is shown below:



Determine which one of the following alternatives describes the change that a catalyst produces to increase the reaction rate.
- **A** Only B is decreased.
- **B** Only A is decreased.
- **C** A, B and C are decreased.
- **D** A and C only are decreased.

7 The following changes are made to a reaction mixture. Determine which one of the following changes will lead to a decrease in reaction rate.
- **A** Smaller solid particles are used.
- **B** The temperature is decreased.
- **C** A catalyst is added.
- **D** The concentration of an aqueous reactant is increased.

8 The schematic diagram below depicts the substitution reaction between chloromethane and a hydroxide ion (OH^-). In this reaction, a Cl atom (green) on the carbon atom is substituted for OH^- (red and white ion).
Using collision theory, explain why collision 1 might be successful, while collisions 2–4 will not be successful.



9 Explain why the rate of reaction between 1 M $CuSO_4$ and powdered zinc is greater than that with an equal mass of large zinc pieces.

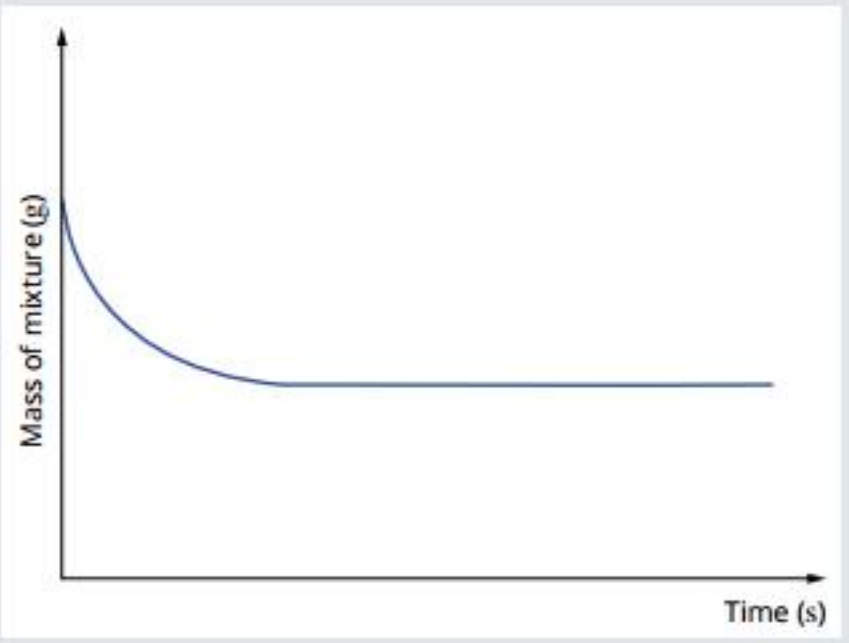
10 Summarise what must occur when reactant particles collide and react.

Analyse

11 **a** Compare the average rate of reaction with the instantaneous rate of reaction.
b Identify how the instantaneous rate and initial rate are similar.

12 Calcium carbonate ($CaCO_3$) chips and 2 M HCl were the starting reactants for the chemical reaction represented by the following chemical equation:
$2HCl(aq) + CaCO_3(s) \rightarrow CaCl_2(aq) + H_2O(l) + CO_2(g)$
Predict what will happen to the rate of reaction (and give your reasons) if the following changes are made to the starting reactants.
a $CaCO_3$ chips and 1 M HCl
b $CaCO_3$ powder and 2 M HCl
c $CaCO_3$ powder and 1 M HCl

13 A 5.00 g piece of copper was dissolved in a beaker containing 500 mL of 2.00 M nitric acid. The equation for the reaction that occurred is:
$3Cu(s) + 8HNO_3(aq) \rightarrow 3Cu(NO_3)_2(aq) + 2NO(g) + 4H_2O(l)$
The changing mass of the mixture was observed for a period of time, and the graph is shown below:



a Identify why the mass of the mixture initially decreases with increasing time.
b Based on the information provided, determine which reactant is limiting.
c Redraw the above graph, then sketch in the expected curve if 500 mL of 1.00 M nitric acid had been used instead. Label your new graph line. Identify why there is a difference in shape.
d Redraw the above graph, then sketch in the expected curve if 5.00 g of powdered copper had been used instead. Label this new graph line. Identify why there is a difference in shape.

14 A reaction is represented by the following chemical equation:

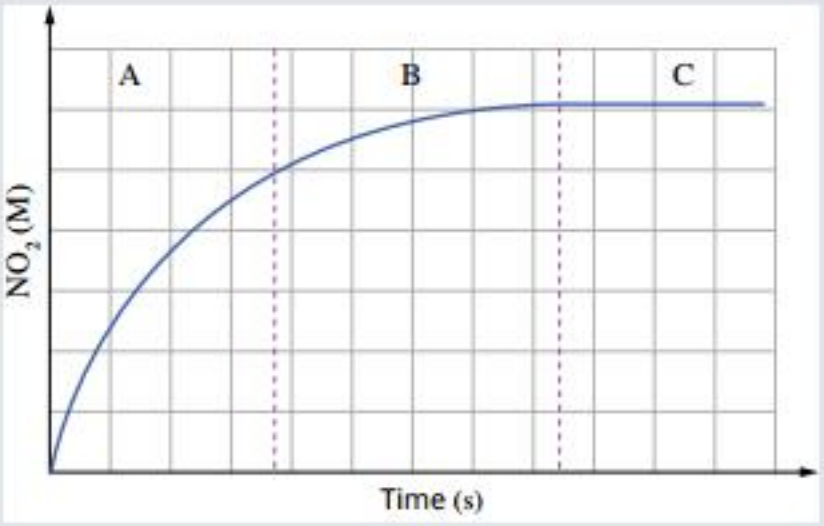
$$3A + B \rightarrow 2C$$

a Create rate expressions for the rate of disappearance of A, the rate of disappearance of B and the rate of appearance of C.
b Using the rate expressions you wrote down in part **a**, if you calculated the average rates of appearance and disappearance over the same time period, predict whether the rates will be equal. If not, rank the rates in order from fastest to slowest.
c If your answer to part **b** was no, create rate expressions for all three substances that would be equal.

15 The production of nitrogen dioxide, NO_2, from nitric oxide, NO, can be represented by the following chemical equation:

$$2NO(g) + O_2(g) \rightarrow 2NO_2(g)$$

A concentration–time curve for the production of NO_2 is shown below:



a Deduce which region of the curve shows a constant value for the rate of reaction—A, B or C. Justify your answer.

b Which region of the curve indicates the fastest rate—A, B or C. Justify your answer.

16 The following data was obtained for the decomposition of hydrogen peroxide, H_2O_2:

Time (s)	$[H_2O_2]$ (M)
0.0	0.600
10.0	0.300
20.0	0.150
30.0	0.0750

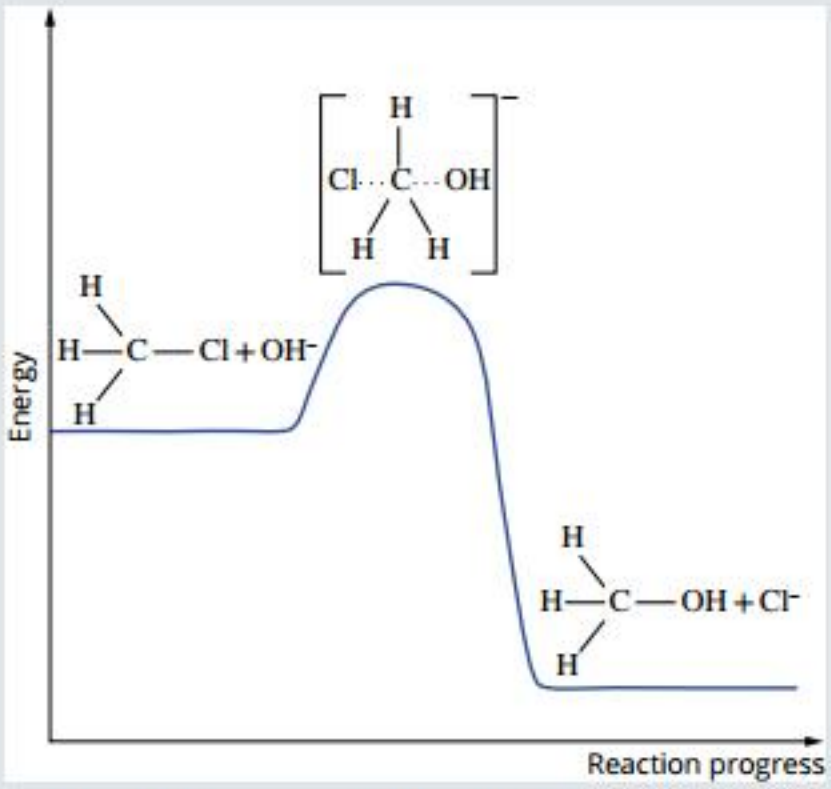
The balanced chemical equation for this chemical reaction is: $2H_2O_2 \rightarrow 2H_2O + O_2$

a Calculate the average rate of disappearance of H_2O_2 between 10.0 s and 20.0 s.

b Calculate the average rate of reaction between 10.0 s and 20.0 s.

c Compare and contrast these measures of rate.

17 The figure below is an energy profile diagram for the substitution reaction between chloromethane and hydroxide ion.



a Copy this diagram and label ΔH and the activation energy.

b Explain what is meant by the term 'activation energy'.

c Predict whether the reaction is endothermic or exothermic.

d Deduce where the transition state occurs and label this position on your diagram.

e Identify the bonds that are beginning to be broken and formed to produce the transition state.

18 Compare and contrast homogeneous catalysts and heterogeneous catalysts. Identify if enzymes are homogeneous or heterogeneous catalysts (or both).

19 The decomposition of hydrogen peroxide can be represented by the following chemical equation:

$$2H_2O_2(aq) \rightarrow 2H_2O(l) + O_2(g)$$

For each of the following, predict whether the rate of reaction will increase or decrease. Provide an explanation in each case.

a decreasing the concentration of hydrogen peroxide

b increasing the temperature

c adding a potassium iodide catalyst

20 **a** Identify the five factors that influence the rate of a reaction.

b Classify the five factors from part **a** according to whether they increase the proportion of successful collisions by:

i increasing collision frequency

ii increasing the proportion of collisions that have energy equal to or greater than the activation energy

21 The Haber process involves the reaction of nitrogen gas and hydrogen gas to make ammonia gas. Identify two ways the rate of this reaction could be increased, at constant temperature. Using collision theory, explain why the rate is increased in each case.

22 Lumps of limestone, calcium carbonate, react readily with dilute hydrochloric acid. Four large lumps of limestone, total mass 10.0 g, were reacted with 100 mL 0.100 M acid.

a Create a balanced equation to represent the reaction

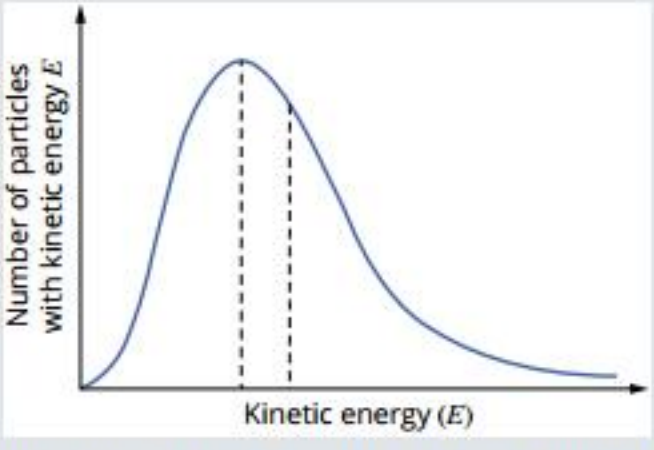
b Identify which reactant is in excess. Use a calculation to support your answer.

c Describe a technique that you could use in a school laboratory to measure the rate of the reaction.

d A 10.0 g sample of small lumps of limestone will react at a different rate from four large lumps. Predict if the rate of reaction with the smaller lumps will be faster or slower. Explain your answer in terms of collision theory.

e Predict two other ways in which the rate of this reaction can be altered. Explain your answer in terms of collision theory.

23 Describe the key features of the Maxwell–Boltzmann plot shown below (for example, axes, data trend). Explain why there are two dashed lines for activation energy.



24 When considering the reaction stage before transition stage (collision of reactants) and the stage after transition stage (formation of products), these can be described as:

A exothermic then endothermic

B endothermic then exothermic

25 According to collision theory, a successful chemical reaction requires:

A a sufficient number of collisions, correct profile, correct volume

B sufficient number of collisions, correct orientation, correct profile

C correct orientation, sufficient energy, sufficient number of collisions

D correct orientation, correct number of collisions, correct pressure

26 Activation energy is equivalent to the:

A energy required to break bonds in products

B energy required to form bonds in reactants

C energy released when bonds are formed in products

D energy required to break bonds in reactants

27 Identify the incorrect statement. A catalyst:

A can be a transition metal or an enzyme

B reacts and is permanently changed during the reaction

C provides an alternate pathway for the reaction

D lowers the activation energy of the reaction

Interpret

28 Airbags in vehicles are a vital safety feature. The chemical reaction in an airbag has which of the following characteristics? (More than one answer is possible.)

A produces significant amounts of heat

B produces significant amounts of gas

C proceeds slowly

D proceeds quickly

29 Hydrogen reacts explosively with oxygen to form water and produces heat.

a Decide what chemical bonds are broken in the reaction.

b Decide what chemical bonds are formed.

c Develop an explanation for how the energy changes during bond breaking and bond forming affect the overall energy change for the reaction.

d Why is there no reaction until the reaction mixture is ignited?

30 The reaction between sodium thiosulfate solution ($Na_2S_2O_3$) and hydrochloric acid solution (HCl) results in the formation of solid sulfur (S), sulfur dioxide gas (SO_2), sodium chloride (NaCl) and water (H_2O).

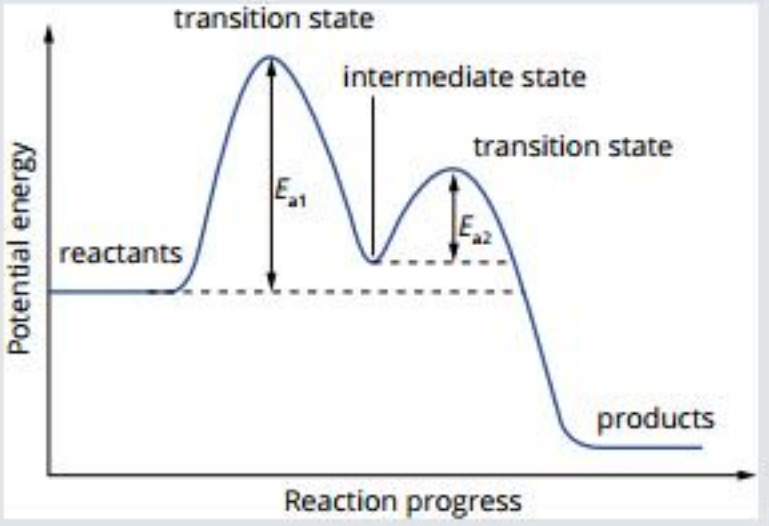
a Develop a balanced chemical equation for this reaction.

b Predict one way in which, experimentally, the course of this reaction can be monitored over time.

c Predict the effect an increase in temperature would have on the rate of reaction.

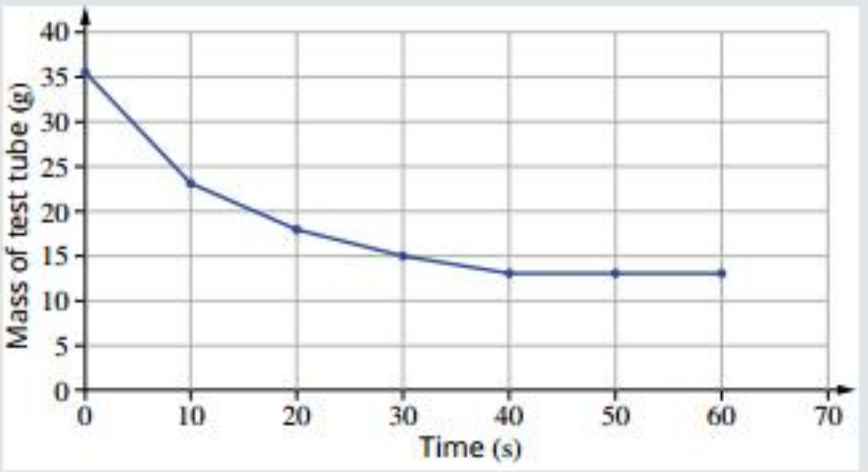
d Predict the effect an increase in HCl concentration would have on the rate of the reaction.

31 A chemical reaction has 2 stages:
Reaction 1: A + B → C + D
Reaction 2: C + D → E + F
The energy profile of the reaction is shown below.



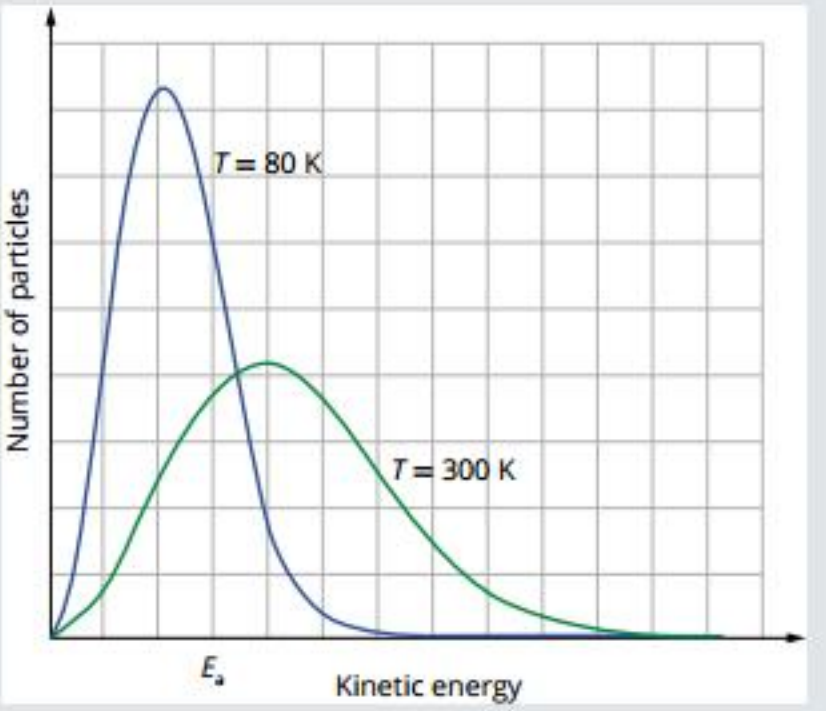
a Determine the species (A to F) present at the reactant, intermediate and product stages in the reaction.
b Describe if the chemical reaction is endothermic or exothermic.

32 The data shown in the following graph was obtained for an acid–metal reaction using hydrochloric acid and a strip of magnesium metal.
a Identify the reason for the decrease in mass of the test tube.
b Calculate the average rate of mass decrease during the first 30 seconds.
c Propose a change to the method or materials that would increase the rate of the reaction.



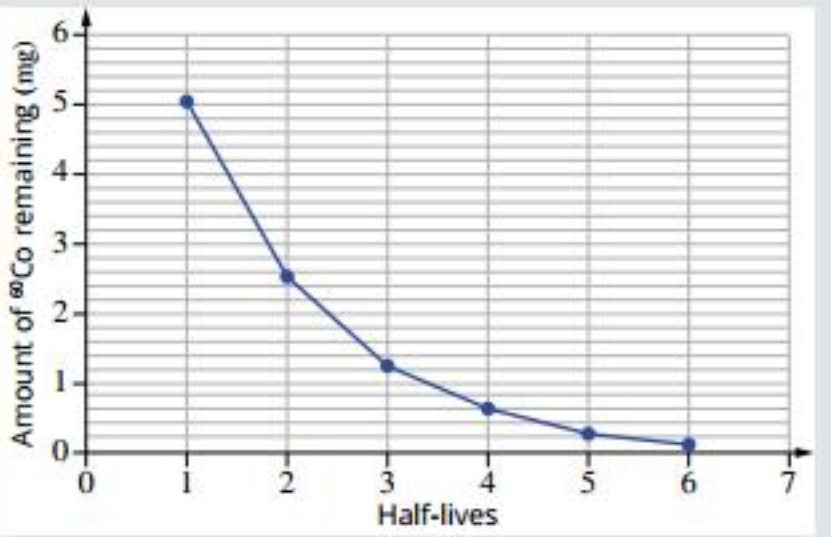
33 Explain your answer to Question 32 (c) using collision theory.

34 The Maxwell–Boltzmann plot for a substance taking part in a reaction is shown below. The activation energy for the substance is labelled.



a Use the data to describe the expected difference in reaction rate at 80 K and 300 K.
b Use collision theory to explain the expected difference in reaction rate between 80 K and 300 K.

35 ^{60}Co is the longest-lived radioactive isotope of cobalt—its half-life is about 5 years. The graph below shows the radioactive decay of ^{60}Co.



a Describe the change to the rate of radioactive decay of cobalt-60 over time.
b Calculate the rate of decay during its second half-life.

Data analysis

DATA SET 1

The information below applies to Questions 1–3.

The gas produced during a reaction of hydrochloric acid and sodium bicarbonate was collected. Four experiments were performed, using high and low acid concentrations at two different temperatures. The same amount of sodium bicarbonate and same volume of acid were used for each experiment. Recording was stopped after 25 minutes irrespective of whether the reaction was finished. Results are shown below.

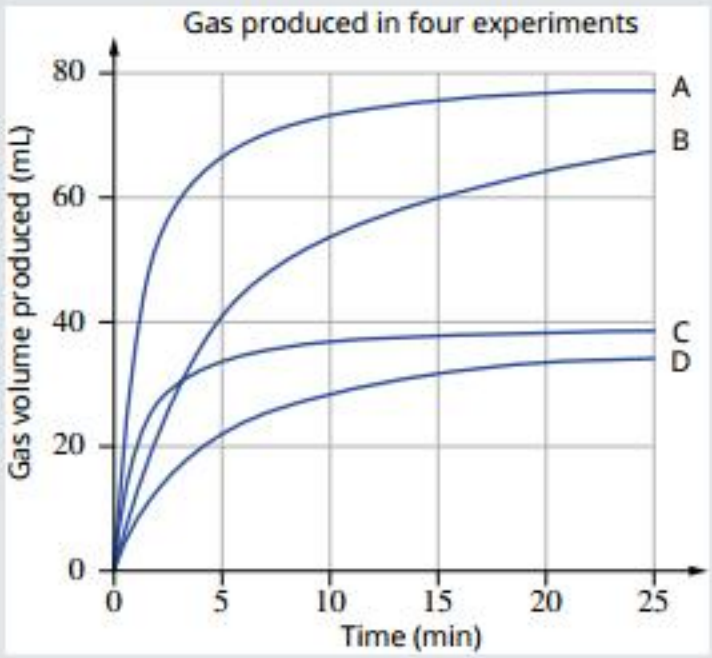


FIGURE 1 Volume of gas produced in four experiments with hydrochloric acid and sodium bicarbonate

Question 1 (2 marks)

Deduce the difference between the reaction conditions of A and C.

Question 2 (2 marks)

Describe the relative amount of reactants and products for reaction B at the end of the recording period. Propose a value for the final gas volume when reaction B is complete.

Question 3 (2 marks)

Determine the average rate of the two low-temperature reactions during the first 10 minutes.

REVIEW QUESTIONS

Molecular interactions and reactions

Topic 1: Intermolecular forces and gases

Multiple-choice questions

1 Which one of the following gives the correct shape for each of the molecules listed?

	Linear	Bent	Tetrahedral
A	CO_2	H_2S	CH_4
B	H_2	CO_2	NH_3
C	HF	H_2O	NH_3
D	H_2O	NH_3	CH_4

2 Which one of the following groups contains only polar molecules?

A NH_3, H_2S, HCl
B CO_2, CH_4, H_2O
C HF, O_2, H_2
D H_2O, NH_3, CH_4

3 Identify which molecule has dispersion forces as the only intermolecular attraction.

A HF
B OF_2
C NF_3
D CF_4

4 Which one of the following R_f values is not possible in paper chromatography?

A $R_f = 0$
B $R_f = 0.5$
C $R_f = 1.0$
D $R_f = 1.2$

5 The blue food dye used in a packet of lollies is known to be non-polar. A thin-layer chromatogram of the lollies is prepared using a non-polar stationary phase and a polar mobile phase. The blue dye will appear on the chromatogram with a:

A low R_f value as the dye is highly soluble in the mobile phase
B low R_f value as the dye is not highly soluble in the mobile phase
C high R_f value as the dye is not highly soluble in the mobile phase
D high R_f value as the dye is highly soluble in the mobile phase

6 Identify which two intermolecular forces form the bonding between molecules of HBr.

A hydrogen bonding and dispersion forces
B hydrogen bonding and ion–dipole attractions
C dipole–dipole attractions and dispersion forces
D dipole–dipole attractions and hydrogen bonding

7 Which of the following alternatives lists SO_2, N_2, C_3H_8 and C_2H_5OH in order of increasing melting point?

A N_2, C_3H_8, SO_2, C_2H_5OH
B N_2, SO_2, C_3H_8, C_2H_5OH
C N_2, SO_2, C_2H_5OH, C_3H_8
D C_3H_8, N_2, C_2H_5OH, SO_2

8 In which of these compounds would you expect hydrogen bonding to play a significant role in determining the boiling point?

H_2O, C_2H_6, CH_3F, C_2H_5OH, CH_3NH_2

A H_2O only
B H_2O, CH_3F and C_2H_5OH only
C H_2O, C_2H_5OH and CH_3NH_2 only
D all except C_2H_6

9 A gas is confined in a cylinder with a movable piston at one end. Assuming the temperature remains constant, if the piston is pushed in, which one of the following statements about the volume and pressure of the gas is correct?

A The pressure will remain unchanged.
B The pressure will increase because the volume is increasing.
C The pressure will decrease due to the increase in volume.
D The pressure will increase because of the decrease in volume.

10 A flask contains equal masses of two gases, hydrogen and nitrogen, at a temperature of 30°C. Which of the following statements about these gases is NOT correct?

A The average kinetic energy $\left(\frac{1}{2}mv^2\right)$ of the molecules of both gases is the same.
B The average velocity of the H_2 molecules is greater than the average velocity of the N_2 molecules.
C There are more H_2 molecules than N_2 molecules in the flask.
D The pressure exerted by the H_2 molecules in the flask is less than the pressure exerted by the N_2 molecules.

11 Determine which of the following gases would occupy the largest volume.

A 0.10 mol of CO_2 at 50°C and 1.0 kPa pressure
B 0.10 mol of H_2 at 40°C and 1.0 kPa pressure
C 0.20 mol of CH_4 at 50°C and 1.0 kPa pressure
D 0.10 mol of O_2 at 50°C and 0.40 kPa pressure

12 A 1.03 kg mass of a gas occupies 520 L at 155°C and 270 kPa pressure. Determine the approximate molar mass of the gas in $g\,mol^{-1}$.

A 9
B 26
C 32
D 44

13 Given that the density, d, of a substance is given by the formula $d = \frac{m}{V}$ and that M represents molar mass, the density of any gas is given by which formula?

A $d = \frac{R \times T}{P \times M}$
B $d = \frac{P}{R \times T \times M}$
C $d = \frac{R \times T \times M}{P}$
D $d = \frac{P \times M}{R \times T}$

14 A 2.06 kg mass of a gas occupies 1040 L at 155°C and 270 kPa pressure. Determine the approximate molar mass of the gas in $g\,mol^{-1}$.

A 26
B 32
C 38
D 44

15 Pentane undergoes complete combustion to produce carbon dioxide and water according to the equation:

$$C_5H_{12}(g) + 8O_2(g) \rightarrow 5CO_2(g) + 6H_2O(g)$$

Which of the following expressions can be used to determine the volume of carbon dioxide, in L, generated by the reaction of 100 g of pentane at STP?
The molar mass of pentane is $72\,g\,mol^{-1}$.

A $\frac{100 \times 22.7}{5 \times 72.17}$
B $\frac{72.17 \times 3}{22.7 \times 100}$
C $\frac{100 \times 5 \times 22.7}{72.17}$
D $\frac{100 \times 72.17}{5 \times 22.7}$

16 20.0 mL of NH_3 and 20.0 mL of O_2 measured at STP react. This reaction may be represented by the following equation:

$$4NH_3(g) + 3O_2(g) \rightarrow 2N_2(g) + 6H_2O(l)$$

After the reaction, gas volumes are again measured at STP. Calculate the volume of oxygen gas that remains unreacted.

A 0.0 mL
B 5.0 mL
C 15.0 mL
D 20.0 mL

Short-answer questions

1 Select the correct answers from the pairs of words to complete the paragraph about molecules and forces:
Physical properties such as vapour pressure, solubility and boiling point are a result of the strength of *intramolecular forces/intermolecular forces* of which there are *three/four* types. Each is based on *atomic/electrostatic* attraction.

2 Consider the compounds carbon dioxide, CO_2, and hydrogen sulfide, H_2S.
Predict whether or not these compounds are polar or non-polar. Justify your prediction in terms of the nature of bonding within each molecule and the shape of each molecule. Illustrate your answer by using appropriate diagrams.

3 The grid below includes formulas for 12 different substances.

hydrogen sulfide H_2S	graphite C	fluorine F_2
carbon dioxide CO_2	methanol CH_3OH	nitrogen N_2
methane CH_4	ammonia NH_3	chloromethane CH_3Cl
hydrogen fluoride HF	oxygen O_2	ethene C_2H_4

Identify substances from this grid that meet the following descriptions.
Note that:
- the same substance may be used more than once
- a complete answer may require the inclusion of more than one substance.

a with non-polar tetrahedral molecules
b with polar tetrahedral molecules
c with non-polar linear molecules
d with one or more atoms covalently bonded to exactly three other atoms
e molecules are attracted to one another by dispersion forces only
f have intermolecular hydrogen bonds
g have molecules of the same shape as water molecules

4 **a** Describe the intermolecular forces between pure samples of F_2, HF and CH_3F.

b Sort these substances from lowest to highest in the relative order of boiling points. Explain your answer.

5 Copy and complete the table below by drawing the Lewis structures of the molecules listed, either drawing or naming the shape of the molecule, and stating the polarity and intermolecular forces present. All valence shell electron pairs should be represented either as a pair of dots or a line.

Molecule	Lewis structure	Shape	Polar or non-polar	Strongest intermolecular force present
H_2O				
CO_2				

6 Ball-and-stick models of some molecules are shown in the following table. Complete the table by identifying the shape of each molecule, stating the approximate bond angle, and providing an example of a substance whose molecules have the shape indicated.

Ball-and-stick model	Shape	Bond angle	Example

7 A student sets up a paper chromatogram and places a spot of green food dye on the origin. In one experiment, the solvent moved 12 cm and a blue spot moved 9 cm from the origin. When the experiment was repeated with the same mobile and stationary phases, the blue spot moved 15 cm. Determine how far (in cm) from the origin the solvent is likely to be in the second experiment.

8 A student uses paper chromatography to investigate chlorophyll, the green liquid extracted from plant leaves. The student notices samples of chlorophyll extract on a narrow piece of chromatography paper and places the paper in ethanol. Inspection of the chromatogram after 10 minutes shows four discernible spots of orange, green and brown colours. The student repeats the process but this time uses hexane as the solvent. The chromatogram produced shows three spots with different R_f values from the first chromatogram. The student then runs a third chromatogram using a mixture of hexane and ethanol as a solvent and the chromatogram shows six discernible spots.

a What conclusions can the student draw?

b Discuss reasons why chemists sometimes use a mixture of solvents, rather than a pure solvent, on a chromatogram.

c Some, but not all, leaves contain beta-carotene. Explain how the student could modify the procedure to confirm if one of the components of the plant extract is beta-carotene.

d The component of the plant extract that has the highest R_f value is known as chlorophyll *a*. How does the solubility of chlorophyll *a* in the mobile phase compare to that of the other components in the extract?

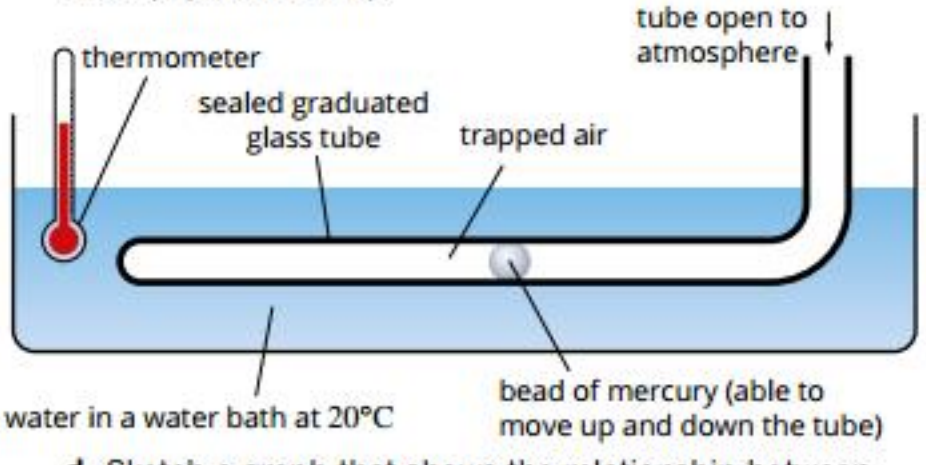
9 Using the kinetic theory of matter, explain why washing hanging on a clothes line will dry faster on a hot day than on a cold day.

10 **a** Use the assumptions of the kinetic theory of gases to explain why raising the temperature of a constant mass of gas, at constant pressure, will result in an increase in the volume occupied by the gas.

b State the conditions under which real gases are *least* likely to obey the gas laws.

c The equipment used to measure the relationship between the volume of a gas and temperature is shown below.

Describe how the pressure would be kept constant in the equipment set-up.


tube open to atmosphere
thermometer
sealed graduated glass tube
trapped air
water in a water bath at 20°C
bead of mercury (able to move up and down the tube)

d Sketch a graph that shows the relationship between pressure (vertical axis) and temperature in degrees Celsius (horizontal axis) for a particular amount of gas at a constant volume.

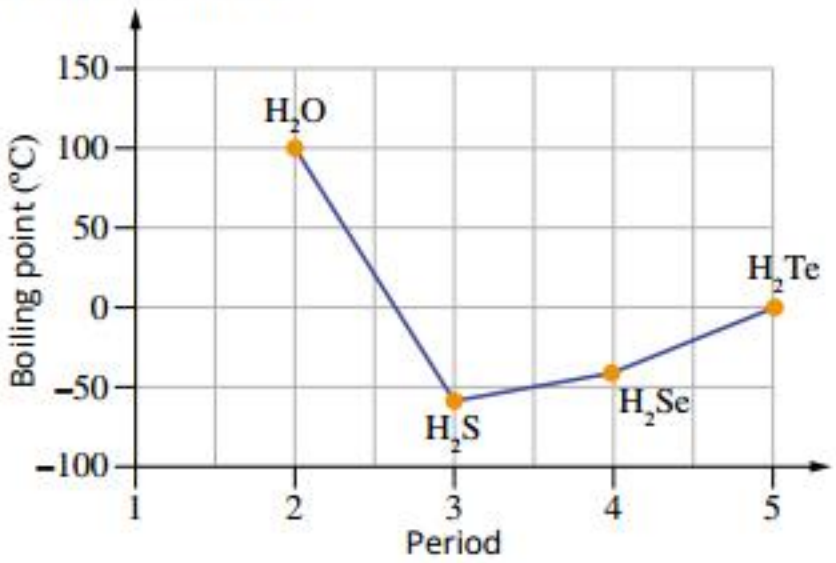
11 A sample of N_2 gas collected at 28.0°C and 98.86 kPa pressure occupies 240.0 mL. Calculate the volume it will occupy at STP.

12 The first step in the industrial manufacture of urea, a widely used fertiliser, is the reaction of ammonia with carbon dioxide at a high temperature and pressure, to form ammonium carbamate:

$$2NH_3(g) + CO_2(g) \rightarrow NH_2COONH_4$$

The ammonium carbamate then decomposes to form urea. If 1.00 kL of ammonia at 210°C and 2.43×10^4 kPa reacts with a slight excess of carbon dioxide to form 177 kg of ammonium carbamate, calculate the percentage yield of this reaction.

13 The following graph shows the boiling points of four group 16 hydrides.



a Explain why the boiling point of H_2S is so much lower than that of H_2O.

b Explain why the boiling point of H_2S is also lower than that of H_2Se.

14 Ammonia (NH_3) is a constituent of many cleaning products for bathrooms.

a Draw an electron dot formula of an ammonia molecule, including non-bonding electron pairs.

b Draw a structural formula for two ammonia molecules, clearly showing the shape of the molecules. Name this shape. On your diagram, label the type of bonds that exist between the:
- atoms within each ammonia molecule
- two ammonia molecules

c Draw a structural formula for a molecule of:
- **i** nitrogen gas
- **ii** carbon dioxide gas

d Explain the following statements.
- **i** The bonds between nitrogen molecules and those between molecules of carbon dioxide are of the same type even though the bonds inside these molecules differ in strength and polarity.
- **ii** The bonds between ammonia molecules are different from those between nitrogen molecules or carbon dioxide molecules.

15 **a** Describe the VSEPR hypothesis.

Consider the following compounds: H_2S, PF_3, $CHCl_3$, CS_2, BF_3.

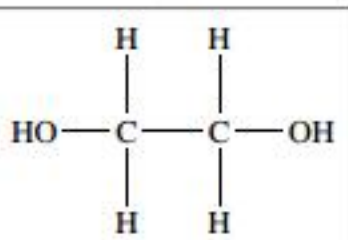
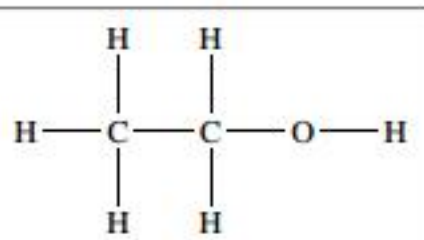
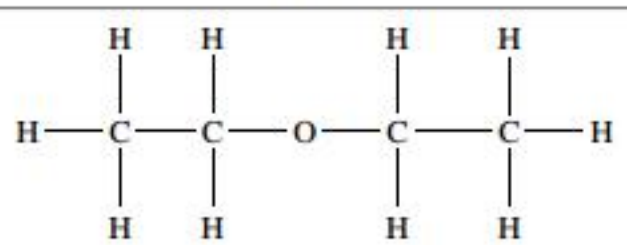
b Explain how the VSEPR hypothesis can be used to determine the shape of each molecule.

c Draw the structure of each compound and include any non-bonding pairs of electrons.

d Identify the shape of each molecule and calculate an approximate value of the bond angle at the central atom.

e Predict if each molecule is polar or non-polar and justify your prediction.

16 Some physical properties and structural formulas of three compounds are provided in the table below.

Compound	Ethane-1,2-diol	Ethanol	Diethyl ether
boiling point at 100 kPa (°C)	197	78	35
vapour pressure at 20°C (kPa)	0.08	0.80	43
molar mass ($g\,mol^{-1}$)	62	46	74
structural formula			

a Vapour pressure is defined as the pressure exerted by a vapour that is in equilibrium with its liquid in a closed container. Describe on the molecular level how this equilibrium is established.

b Explain the relationship between vapour pressure and boiling point.

c Explain the relative order of the following in terms of the molecular structure and the nature of intermolecular forces.

i boiling points

ii vapour pressure of the three compounds

17 Ethane, C_2H_6, and hexane, C_6H_{14}, are similar because both molecules have a structure that comprises a carbon backbone with hydrogen atoms attached. However, the boiling point of ethane is –89°C and the boiling point of hexane is 69°C. Interpret this data in terms of both the intramolecular bonding and intermolecular forces that occur in these compounds.

18 Both hexanol, $CH_3CH_2CH_2CH_2CH_2CH_2OH$, and methanol, CH_3OH, have a polar O–H bond capable of forming hydrogen bonds with water. Explain why methanol is soluble in water, while hexanol is insoluble.

19 A chemist analysed an alloy that contained magnesium, zinc and a small amount of non-metallic impurity. She took a 2.00 g sample of the alloy and divided it into two portions of equal mass.

One of these portions she reacted completely with dilute hydrochloric acid and obtained 0.420 L of hydrogen gas at 22.0°C and 100.0 kPa pressure.

$$Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$$
$$Zn(s) + 2HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$$

The other portion she reacted as completely as possible with sodium hydroxide solution and obtained 0.308 L of hydrogen gas at STP. In this part of the experiment, only the amphoteric metal, the zinc, reacts:

$$Zn(s) + 2OH^-(aq) + 2H_2O(l) \rightarrow Zn(OH)_4^{2-}(aq) + H_2(g)$$

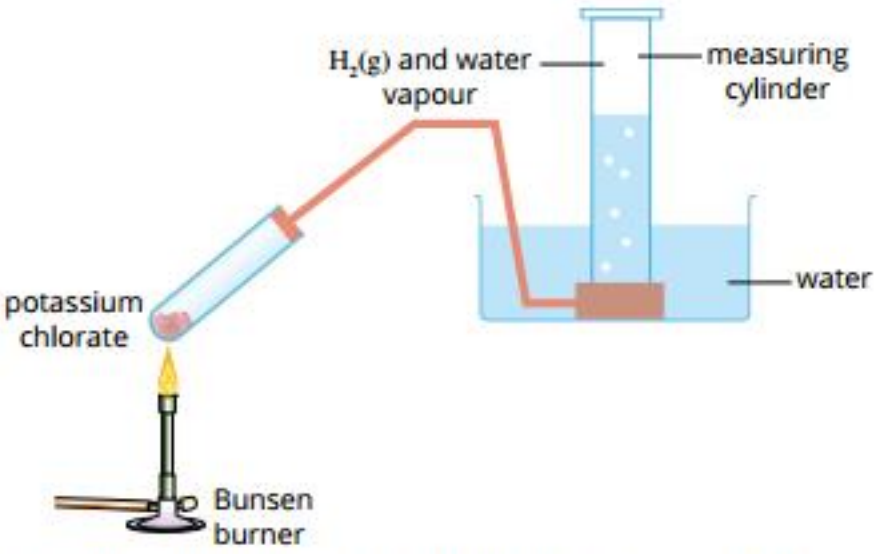
a Use the data from the second experiment to calculate the percentage by mass of zinc in the alloy.

b Use the information from the first experiment to determine the percentage, by mass, of magnesium in the alloy.

c Determine the percentage, by mass, of impurities in the alloy. Assume that the impurities did not react with either hydrochloric acid or sodium hydroxide.

20 The apparatus shown below was used to determine the molar volume of oxygen. The oxygen was generated in the test tube by heating potassium chlorate and collected by the displacement of water in the measuring cylinder.

$$2KClO_3(s) \rightarrow 2KCl(s) + 3O_2(g)$$



The measurements made during the experiment are provided in the following table.

mass of test tube + contents before heating	38.550 g
mass of test tube + contents after heating	38.225 g
volume of gas collected	242.0 mL
atmospheric pressure	99.00 kPa
room temperature	20.0°C
vapour pressure of water at room temperature	2.34 kPa

(For this question, assume the water vapour pressure in the measuring cylinder is negligible.)

a Calculate the pressure of the oxygen gas in the measuring cylinder.

b Determine the number of moles of oxygen produced.

c Calculate the molar volume of the oxygen at the experimental conditions.

d Determine the molar volume of oxygen at STP.

e Calculate the percentage error if the accepted value of the molar volume of a gas is 22.7 L mol^{-1} at STP.

f The introduction to this question stated you could assume the water vapour pressure in the measuring cylinder is negligible. The value is actually 2.34 kPa at room temperature. If this value was included in your calculations, would the percentage error increase or decrease? Justify your answer.

Topic 2: Aqueous solutions and acidity

Multiple-choice questions

1 Which type of bonds hold molecules of water in a crystalline lattice in ice?

A polar covalent bonds only

B hydrogen bonds and dispersion forces only

C polar covalent bonds and hydrogen bonds only

D polar covalent bonds, hydrogen bonds and dispersion forces

2 Identify which of the following statements about solutions are true.

- **i** When sodium chloride is dissolved in water, the water is the solute.
- **ii** An unsaturated solution contains more solute than is needed to saturate it.
- **iii** A supersaturated solution contains less dissolved solid per unit volume than a saturated solution.
- **iv** In general, the solubility of a gas in a liquid decreases with increasing temperature.
- **v** When sodium nitrate dissolves in water, dissociation occurs.

A ii, iii and iv
B i, ii and iv
C ii and v
D iv and v

3 Which one of the following does NOT change when a solution is diluted by the addition of more solvent?

A volume of solvent
B number of moles of solute
C concentration of solution
D mass of solution

4 Select the ionic equation for the reaction that occurs when solutions of barium chloride and sodium sulfate are mixed.

A $Ba^{2+}(aq) + SO_4^{2-}(aq) \rightarrow BaSO_4(s)$
B $2Na^{+}(aq) + SO_4^{2-}(aq) \rightarrow Na_2SO_4(s)$
C $BaCl_2(aq) + NaSO_4(aq) \rightarrow NaCl(aq) + BaSO_4(s)$
D $BaCl_2(aq) + Na_2SO_4(aq) \rightarrow 2NaCl(aq) + BaSO_4(s)$

5 Which of the following pairs of solutions would NOT form a precipitate when mixed together?

A magnesium chloride solution and potassium carbonate solution
B zinc chloride solution and potassium phosphate solution
C calcium chloride solution and copper(II) nitrate solution
D lead nitrate solution and iron(III) iodide solution

6 A solution of sodium hydroxide when added to a solution of aluminium chloride produces a gel-like precipitate. The precipitate reaction could be represented as:

A $Na^{+}(aq) + Cl^{-}(aq) \rightarrow NaCl(s)$
B $Al^{3+}(aq) + 3OH^{-}(aq) \rightarrow Al(OH)_3(s)$
C $Al^{3+}(aq) + 3Cl^{-}(aq) \rightarrow AlCl_3(s)$
D $H^{+}(aq) + OH^{-}(aq) \rightarrow H_2O(l)$

7 You have been provided with three unlabelled beakers containing aqueous solutions of zinc chloride, sodium carbonate and barium nitrate. Select the reagent that could be used to identify each of the solutions.

A dilute nitric acid
B dilute sulfuric acid
C dilute hydrochloric acid
D sodium chloride solution

8 The pH of a 2.0 M propanoic acid solution is measured as 2.9. The solution can be described as:

A a dilute, weak acid
B a dilute, strong acid
C a concentrated, weak acid
D a concentrated, strong acid

9 Which one of the following describes the types of bonds broken in the solute and formed with water when hydrogen chloride dissolves?

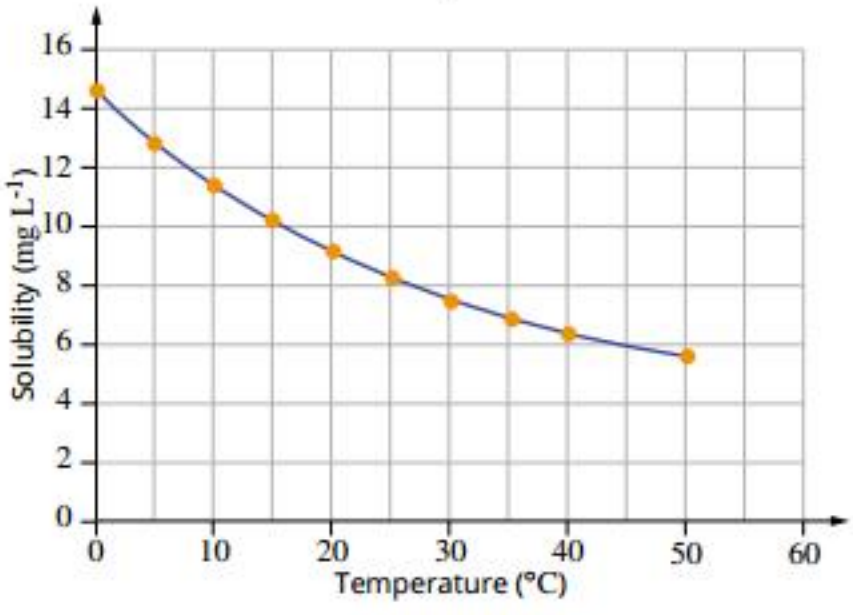
	Bonds broken	Bonds formed
A	covalent	hydrogen and dipole–dipole
B	dipole–dipole	covalent and ion–dipole
C	dipole–dipole	hydrogen and dipole–dipole
D	covalent	covalent and ion–dipole

10 Use the pH value of the solutions listed below to identify the substance that has the highest concentration of H_3O^{+} ions.

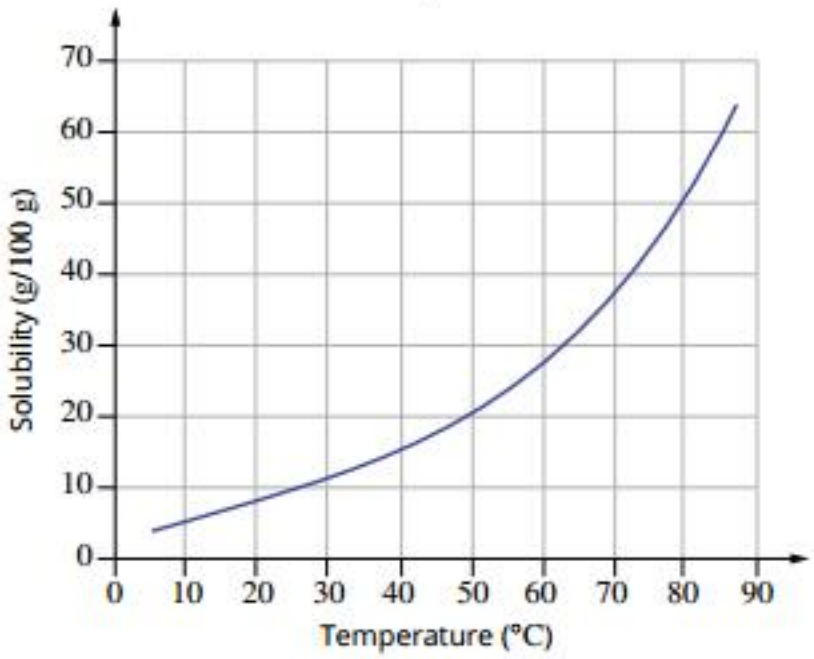
A soap solution pH 9.0
B sea water pH 8.1
C rainwater pH 5.6
D wine pH 3.6

11 Consider the shape of the following solubility curves.

Graph A



Graph B



Select which one of the following alternatives correctly attributes the most likely shape of the solubility curve for the ionic solid potassium chlorate and the gas oxygen.

	Potassium chlorate	Oxygen
A	graph A	graph A
B	graph A	graph B
C	graph B	graph A
D	graph B	graph B

12 Beakers A and B both contain nitric acid. The pH of the acid in beaker A is 3 whereas the pH of the acid in beaker B is 1. From this information, select the correct deduction about the concentration of hydrogen ions in beaker A.

A It is three times that in beaker B.
B It is one-third that in beaker B.
C It is a hundred times that in beaker B.
D It is one-hundredth of that in beaker B.

13 Predict the products of the reaction between iron(II) carbonate and dilute hydrochloric acid.

A H_2O and $FeCl_2$
B H_2 and $FeCl_2$
C H_2, Fe, Cl_2 and CO_2
D CO_2, H_2O and $FeCl_2$

14 Which equation represents the reaction between solid magnesium hydroxide and dilute nitric acid?

A $Mg(s) + 2H_3O^+(aq) \rightarrow Mg^{2+}(aq) + 2H_2O(l) + H_2(g)$
B $Mg^{2+}(aq) + 2NO_3^-(aq) \rightarrow Mg(NO_3)_2(s)$
C $Mg(OH)_2(s) + 2H_3O^+(aq) \rightarrow Mg^{2+}(aq) + 2H_2O(l)$
D $Mg(OH)_2(s) + 2NO_3^-(aq) \rightarrow Mg(NO_3)_2(s) + 2OH^-(aq)$

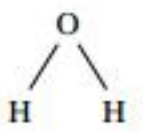
15 The products of a reaction are calcium sulfate and hydrogen gas. The reactants used were:

A calcium metal and sulfuric acid
B calcium metal and hydrogen sulfide
C calcium sulfide and sulfuric acid
D calcium nitrate and sulfuric acid

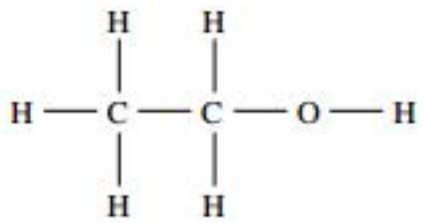
Short-answer questions

1 A student is provided with samples of some liquids that could be either pure liquids or solutions. Propose a simple test that the student could perform to determine which of the liquids are solutions. In your response, assume that standard laboratory equipment such as glassware, Bunsen burner and refrigeration is available.

2 200 g of water is placed in one beaker and 200 g of ethanol in another. Initially, both substances are the same temperature. The specific heat capacity of ethanol is 2.4 Jg^{-1} $°C^{-1}$ and that of water is 4.18 Jg^{-1} $°C^{-1}$. Each beaker is heated by the addition of 5 kJ of heat energy. The molecular structures of water and ethanol are shown below.



water
18 g mol^{-1}



ethanol
46 g mol^{-1}

a How would you expect the temperature of the ethanol to compare to that of the water after heating?
b Propose a reason for these observed differences in temperature increase, making reference to the specific heat capacities and the strength of the bonding that would exist between molecules.

3 **a** Calculate the molar concentration of $FeCl_3$ in a 500 mL sample that contains 0.24 mol.
b Calculate the amount, in moles, of solute in 440 mL of 0.25 M $FeCl_3$.
c Calculate the mass of solute, in grams, of $FeCl_3$ in 1.5 L of 0.50 M solution.

4 After dissolving 5.00 g of table salt (NaCl) in water, a solution is made up to 200 mL with water.

a Write a chemical equation to represent this process.
b Draw a labelled diagram to show the arrangement of water molecules around the dissolved sodium ions and chloride ions.
c Calculate the molar concentration of the solution.
d Explain why ice floats on water.
e Explain the term 'surface tension' and describe how it arises in water.

5 A student has three solutions of potassium chlorate ($KClO_3$). One is unsaturated, one is saturated and one is supersaturated.

- **a** Define the term 'saturated'.
- **b** Devise and describe a simple method that could be used to determine which solution is which. Describe the results you would expect for each solution.
- **c** A solution of potassium chlorate is made by dissolving 5.67 g of the solid in distilled water to make up 250.0 mL of solution. The molar mass of $KClO_3$ is 122.6 g mol^{-1}.
  - **i** Calculate the concentration of this solution in g L^{-1}.
  - **ii** Calculate the concentration of this solution in mol L^{-1}.
  - **iii** If this solution is added to a beaker containing 350 mL of water, determine the concentration of the diluted solution in mol L^{-1}.

6 A pair of chemistry students investigated the solubility of potassium nitrate, KNO_3, in water. They weighed out 25 g of water into a test tube and then heated the test tube and contents to 60°C in a beaker of hot water. They then weighed out 13.0 g of potassium nitrate and dissolved it, while stirring it, in the water in the test tube. The students then took the test tube out of the hot water and allowed it to cool, stirring the solution gently with a thermometer. Small crystals of potassium nitrate first appeared when the temperature of the solution had cooled to 35°C.
According to the students' results, what is the solubility of potassium nitrate in g/100 g water at 35°C?

7 Calculate the volume of water, in mL, that must be added to 20.0 mL of 0.5 mol L^{-1} NaCl to change its concentration to 0.20 mol L^{-1}.

8 25.0 mL of a 0.30 M potassium sulfate solution and 40.0 mL of a 0.40 M potassium sulfate solution were added together and mixed thoroughly in an empty beaker.

- **a** Calculate the final concentration of potassium sulfate in the new beaker.
- **b** Calculate the concentration of potassium ions in the new beaker.

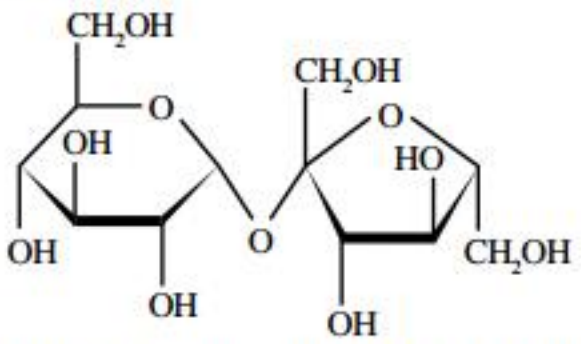
9 Some excess potassium chloride solution is added to a solution containing 3.15 g of lead(II) nitrate. A white precipitate forms.

- **a** Write a full chemical equation for the formation of the precipitate.
- **b** Write an ionic equation for the formation of the precipitate.
- **c** For this reaction, give the name of the:
  - **i** precipitate
  - **ii** spectator ions
- **d** Assume there was sufficient potassium chloride to react with all of the lead(II) nitrate.
  - **i** Calculate the number of moles of lead(II) nitrate that reacted.
  - **ii** Calculate the mass of precipitate that would form.

10 You are given five solutions. They are not labelled but are known to be sodium carbonate, sulfuric acid, potassium nitrate, magnesium nitrate and copper(II) nitrate. You have been set the task to identify the solutions.

- **a** Predict what you would observe if a sample of each solution was added to a sample of each of the other four solutions. (If no observable reaction is predicted, write 'no change'.)
  - **i** sodium carbonate and sulfuric acid
  - **ii** sodium carbonate and potassium nitrate
  - **iii** sodium carbonate and magnesium nitrate
  - **iv** sodium iodide and copper(II) nitrate
  - **v** sulfuric acid and potassium nitrate
  - **vi** sulfuric acid and magnesium nitrate
  - **vii** sulfuric acid and copper(II) nitrate
  - **viii** potassium nitrate and magnesium nitrate
  - **ix** potassium nitrate and copper(II) nitrate
  - **x** magnesium nitrate and copper(II) nitrate
- **b** Write a balanced ionic equation for each of the reactions predicted in part **a**.
- **c** Describe how the solutions can be identified by mixing each solution with each of the other four solutions.

11 Common salt (sodium chloride, NaCl) is an ionic compound. Table sugar (sucrose, $C_{12}H_{22}O_{11}$) is a covalent molecular compound. The structure of sucrose is provided.



Both of these substances are highly soluble in water yet the solution processes for these substances are different. Give a brief description of the solution process for the following items.

- **a** common salt
- **b** sugar

12 Describe what happens at the molecular level during the neutralisation of an acid with a base. Use an example to assist in your description and write full and ionic equations for your chosen neutralisation reaction.

13 Write the balanced chemical equation and the ionic equation for the reaction between magnesium (Mg) and sulfuric acid (H_2SO_4).

14 Explain how the pH of a solution changes when a strong acid is diluted. What effect does this have on the hydronium ion concentration, and how can this be demonstrated mathematically?

15 When dilute sulfuric acid is added to substance A (a solid), there is a vigorous effervescence and the gas explodes when ignited in air. When the remaining solution is concentrated, colourless crystals separate. A confused student identifies these crystals as magnesium oxide, zinc sulfate or calcium oxide.

- **a** Determine the identity of the crystals. Explain your reasoning.
- **b** Identify the metal and explain your answer.
- **c** Write a balanced chemical equation to show the reaction of A with dilute sulfuric acid.

16 Determine the pH of the following solutions.

- **a** 0.001 M HCl
- **b** 0.5 M HNO_3
- **c** 0.01 M LiOH

17 20 mL of 0.1 M HCl is added to a beaker. A small amount of phenolphthalein indicator is also added. Droplets of 1.0 M NaOH are allowed to drip into the HCl at even intervals.

- **a** Calculate the pH of the HCl before any HCl is added.
- **b** Describe how the pH will change over time.
- **c** Will the pH change in a linear fashion?
- **d** How will the colour of the solution change?

18 A 0.20 mol sample of hydrogen chloride gas is bubbled into 300.0 mL of distilled water to produce an acidic solution. The 300.0 mL of solution is divided evenly into three 200 mL flasks.

- **a** Write the full equation and an ionic equation for the reaction that occurs when a short length of magnesium is added to the first flask.
- **b** An 80.0 mL volume of 1.0 M silver nitrate solution ($AgNO_3$) is added to the second flask. A white solid forms.
  - **i** Write an ionic equation to explain the appearance of the white solid.
  - **ii** Following the addition of the silver nitrate solution, predict if any hydrogen chloride will remain in the mixture. Explain your answer with the aid of relevant calculations.
- **c** A small amount of copper(II) carbonate is added to the third flask.
  - **i** Describe the expected observations.
  - **ii** Write full and ionic equations to account for these observations.

19 The health authorities in Australia recommend the safe level of lead in drinking water to be 0.01 ppm. Despite lead and its compounds being very toxic, products used every day, such as car batteries, still contain lead. Lead and many of its compounds are insoluble in water, so it is assumed that very little lead enters the drinking water supply by the dissolution of lead substances.

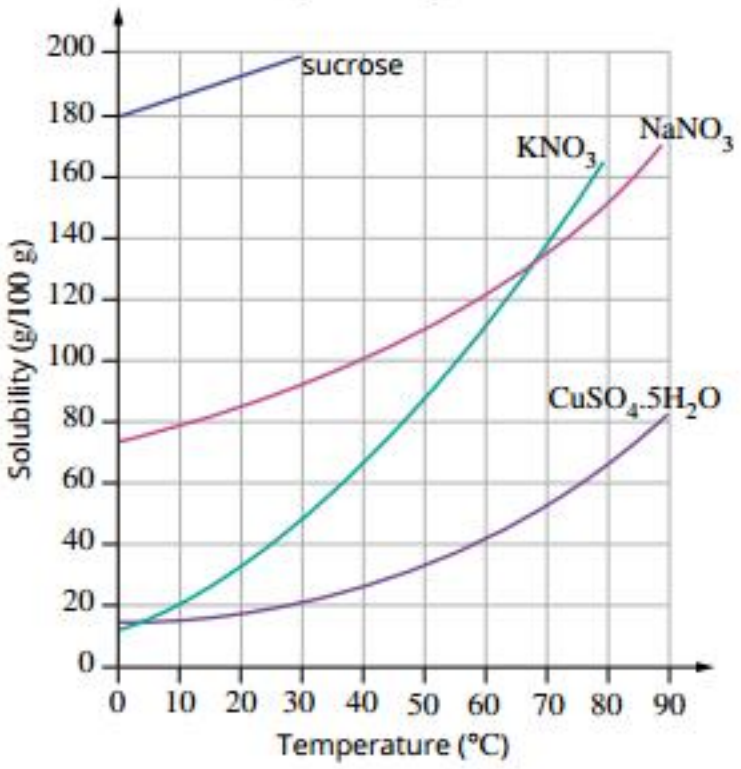
Lead(II) oxide, a compound regarded as insoluble in water, is used to make crystal glassware and as a pottery glaze. The solubility of lead oxide at 25°C is 0.002 g per 100 g of water. If some water is stored in a 1.0 L bowl of crystal glass, determine whether this water could possibly dissolve sufficient lead oxide to raise the level of lead in the water over the recommended safe level.

20 The solubilities of three different substances at 20°C and 80°C are given in the table below.

Substance	Solubility in water (g per 100 g water)	
	20°C	80°C
potassium sulfate	12.0	21.0
sodium chloride	36	37
graphite	insoluble	insoluble

- **a** If 16.0 g of sodium chloride and 50 g of water were mixed, determine what mass of sodium chloride would dissolve at 20°C.
- **b** If 9.0 g of potassium sulfate and 50 g of water were mixed, determine what mass of potassium sulfate would dissolve at:
  - **i** 20°C
  - **ii** 80°C
- **c** If 1.5 g of graphite and 50 g of water were mixed, determine what mass of graphite would dissolve at 20°C.
- **d** Determine the solubility of potassium sulfate at 20°C expressed in mol L^{-1}. The density of water at 20°C is 1.00 g mL^{-1}. Assume that the volume of the solution is equal to the volume of water.
- **e** You are given a mixture that contains 16.0 g of sodium chloride, 9.0 g of potassium sulfate and 1.5 g of graphite.
  - **i** Describe how you could obtain a pure sample of potassium sulfate and a pure sample of graphite from this mixture.
  - **ii** Determine the maximum mass of potassium sulfate that could be obtained by this method.
- **f** Use the data provided in the table above to explain why it would be difficult to obtain a pure sample of sodium chloride from the mixture.

21 Consider the following solubility curves.



a **i** Determine the minimum mass of $NaNO_3$ that must be dissolved in 100 g of water to produce a saturated solution at 50°C.

ii Predict what would be observed if the solution in part **i** were cooled to 20°C.

iii Determine what mass of water must be added to 110 g of $NaNO_3$ to make a saturated solution at 10°C.

b Determine the maximum amount of table sugar (sucrose) that can dissolve in a cup containing 200 g of water at 30°C.

c Three different solutions of KNO_3 are prepared by adding various masses of KNO_3 to 100 g of water. All three solutions are maintained at 50°C.

The masses of KNO_3 contained in the solutions are 30 g, 80 g and 87 g.

i Use this information to clearly explain the differences between a saturated solution, an unsaturated solution and a supersaturated solution.

ii Describe a simple test that you could use to identify which solution is which.

iii Predict what would happen to each solution if it was cooled to 30°C.

d Determine what mass of water must be added to 35 g of $CuSO_4 \cdot 5H_2O$ to make a saturated solution at 20°C.

22 In 1887, the Swedish scientist Svante Arrhenius developed a model that explains some of the properties of acids and bases.

a Describe how acids and bases are defined in the Arrhenius model.

b The results of a student investigation into some properties of strong and weak acids are summarised in the table below.

Explain, in terms of the Arrhenius model, the difference in pH, and reactivity between the two acids.

Properties of strong and weak acids

Property	Hydrochloric acid, HCl	Ethanoic acid, CH_3COOH
volume of acid solution	20.0 mL	20.0 mL
concentration of acid	0.10 mol L^{-1}	0.10 mol L^{-1}
pH	1.0	3.0
electrical conductivity	high	low
reactivity with sodium carbonate solution	fast	slow

c In a follow-up experiment, the students found that 10.0 mL of 0.20 mol L^{-1} sodium hydroxide solution was required to neutralise the hydrochloric acid solution. Predict if you would expect the volume of sodium hydroxide required to neutralise the ethanoic acid solution to be less than or equal to 10.0 mL. The concentration of base used in the two neutralisation reactions is the same. Explain your answer.

Topic 3: Rates of chemical reactions

Multiple-choice questions

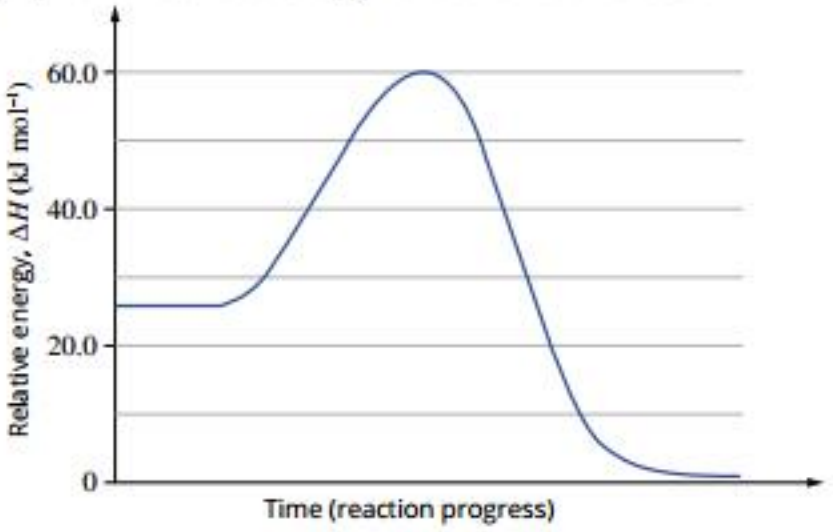
1 Which one of the following will NOT increase the initial rate of the reaction between 0.2 g of $CaCO_3$ and 100 mL of 0.1 M hydrochloric acid?

A crushing the $CaCO_3$
B using a larger volume of the acid
C increasing the temperature of the acid
D using more concentrated acid

2 Consider the statement: 'The rates of all chemical reactions increase with a rise in temperature.'
Identify which one of the following is correct.

A This statement is true, since the activation energies for all reactions increase with a rise in temperature.
B This statement is false, since the rate of an exothermic reaction decreases with a rise in temperature.
C This statement is false, since the rate of an endothermic reaction decreases with a rise in temperature.
D This statement is true, since a greater proportion of molecular collisions will result in reaction.

The following information relates to Questions **3** and **4**.
The graph shows the enthalpy for a chemical reaction.



3 What are the values for the enthalpy change, ΔH, and the activation energy, E_a, in $kJ\,mol^{-1}$ for the reaction?

A $\Delta H = -25\,kJ\,mol^{-1}$ and $E_a = 35\,kJ\,mol^{-1}$
B $\Delta H = +25\,kJ\,mol^{-1}$ and $E_a = 35\,kJ\,mol^{-1}$
C $\Delta H = 35\,kJ\,mol^{-1}$ and $E_a = 60\,kJ\,mol^{-1}$
D $\Delta H = -60\,kJ\,mol^{-1}$ and $E_a = 35\,kJ\,mol^{-1}$

4 Predict what will happen if a catalyst is added to the system.

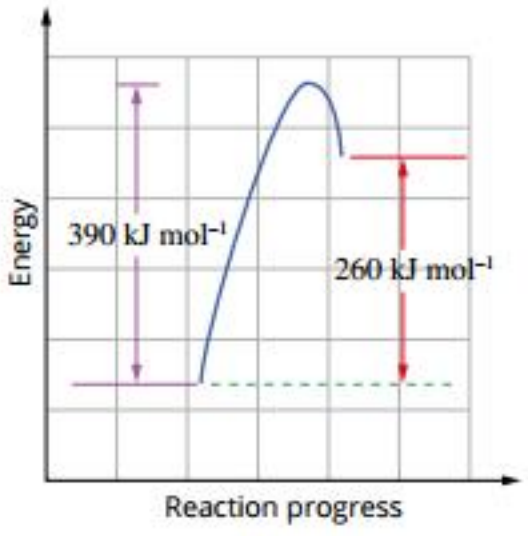
A Both ΔH and E_a will decrease.
B ΔH will remain constant but E_a will decrease.
C ΔH will decrease and E_a will remain constant.
D Both ΔH and E_a will remain constant.

5 Select the alternative that explains why the rate of a chemical reaction decreases as the reactions proceeds.

A The reactant concentrations decrease with time.
B A catalyst is needed to maintain a constant rate of reaction.
C The proportion of reactant molecules with energies in excess of the activation energy decreases as the reaction proceeds.
D Heat energy must be added to maintain the reaction rate.

The following information relates to Questions **6** and **7**.
The energy profile diagram shown is for the following reaction.

$$CO_2(g) + NO(g) \rightarrow CO(g) + NO_2(g)$$



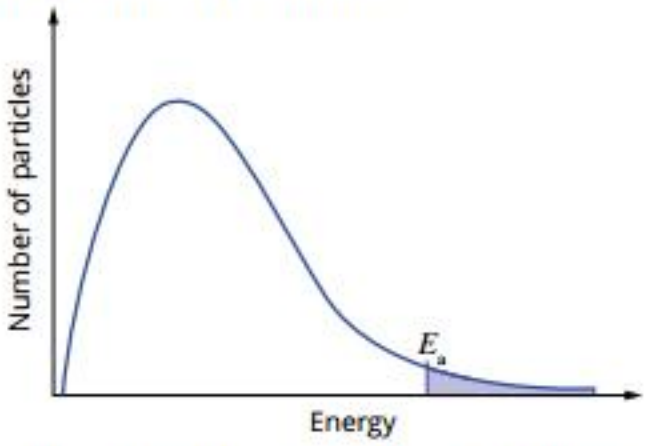
6 Determine the ΔH of the forward reaction, in $kJ\,mol^{-1}$.

A −130
B +130
C +230
D +260

7 Determine the activation energy of the reverse reaction, in $kJ\,mol^{-1}$.

A 40
B 130
C 230
D 360

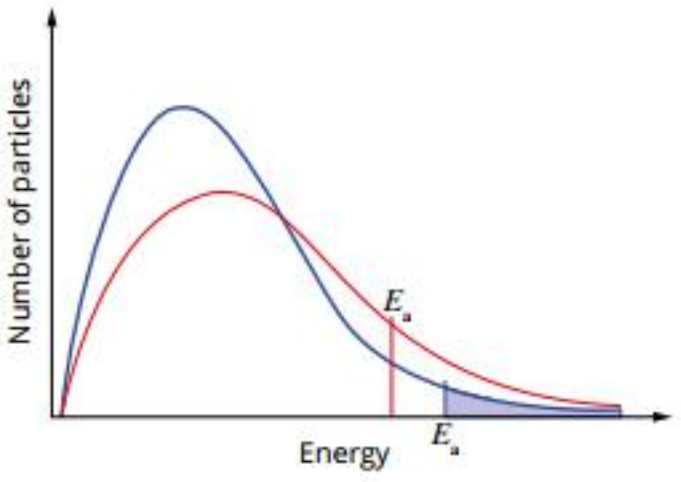
8 The diagram below shows the typical Maxwell–Boltzmann distribution of kinetic energies of the particles in a reaction mixture.



If E_a represents the activation energy for the reaction, identify what the shaded area represents.

A the total amount of energy that will be released during the reaction
B the proportion of reactant particles that are moving fast enough at a given instant for a collision to result in the formation of products
C the energy that must be added to the reactant mixture to initiate the reaction
D the proportion of reactant particles with the correct orientation to react

9 Two changes are made to the reaction mixture from Question **8**, affecting both the distribution curve and the activation energy, as shown in red in the diagram below.



Which of the following gives changes in conditions that are consistent with these effects?

	Change in distribution curve	Change in activation energy
A	higher temperature	catalyst added
B	higher temperature	lower pressure
C	higher pressure	lower temperature
D	higher pressure	catalyst added

10 Which of the following statements about a catalyst is NOT true?

A A catalyst is not consumed in the course of a reaction.
B A catalyst alters the reaction pathway between reactants and products.
C A catalyst reduces the energy released or absorbed by a reaction.
D The proportion of molecules with sufficient energy to react is increased by a catalyst.

11 The equation for the decomposition of hydrogen peroxide is:

$$2H_2O_2(l) \rightarrow 2H_2O(l) + O_2(g)$$

This is a relatively slow reaction that can be catalysed by the addition of manganese dioxide or by the addition of pieces of liver from animals. There is an enzyme in liver that catalyses the reaction.
Two experiments with hydrogen peroxide and MnO_2 are conducted.

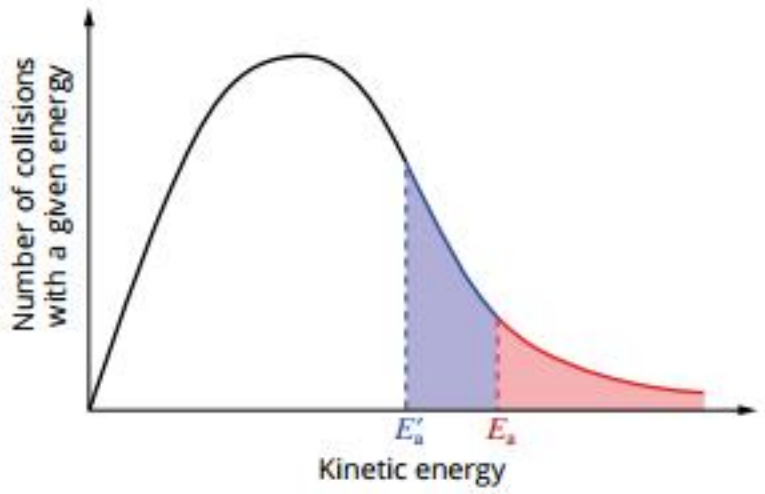
Experiment 1	Experiment 2
100 mL of H_2O_2 with one spatula of MnO_2	100 mL of H_2O_2 with two spatulas of MnO_2

Both reactions are monitored until no further reaction occurs.
Select the correct statement comparing the two experiments.

A Experiment 2 will produce twice the volume of oxygen gas.
B The volume of oxygen gas will depend upon which chemical is in excess.
C Both reactions produce the same volume of oxygen gas but at different rates.
D The rate of reaction will be the same in both flasks.

12 In the following Maxwell–Boltzmann distribution curve:

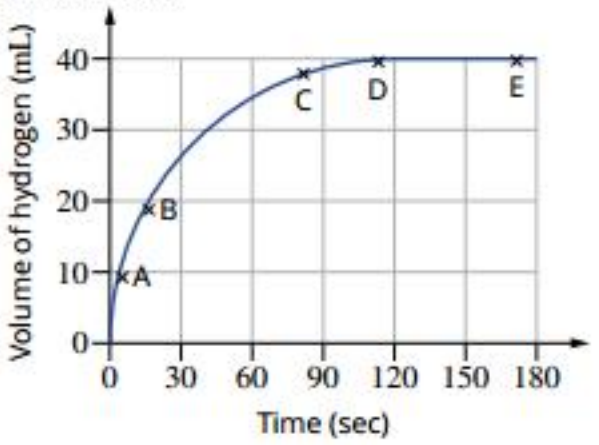
- E_a represents the activation energy for an uncatalysed reaction.
- E_a' represents the activation energy for the catalysed reaction.



Select the coloured region under the graph that represents the number of particles with sufficient energy to lead to the successful formation of products in a catalysed chemical reaction.

A blue only
B white only
C blue and pink only
D white and blue only

13 Refer to the following graph, which shows the volume of hydrogen produced against time during a rate of reaction experiment between zinc and dilute hydrochloric acid.



Determine the point in the graph at which the reaction rate is the greatest.

14 The effect of decreasing the particle size of a solid reactant is to:

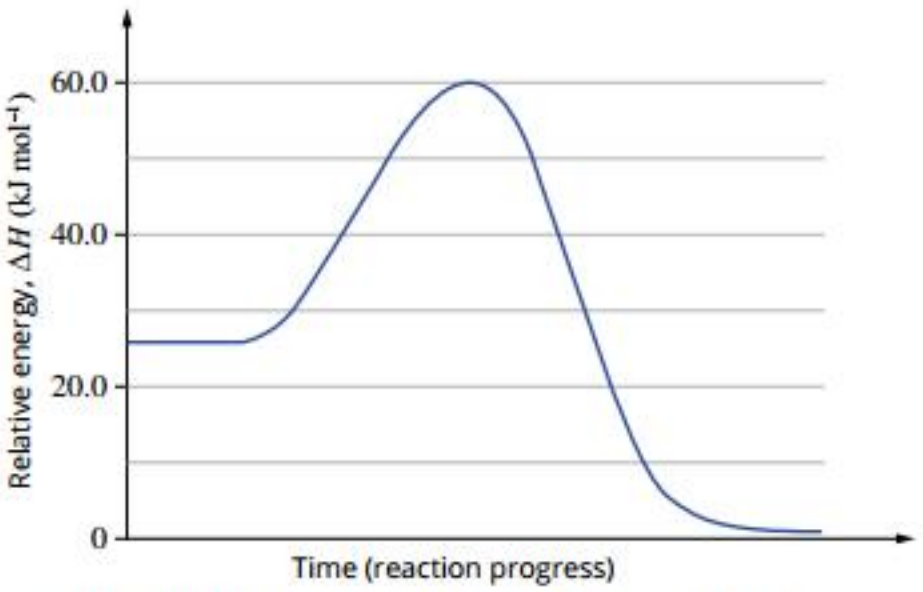
A decrease the number of collisions
B increase the number of collisions
C increase the energy of collisions
D increase the energy of collisions and decrease the number of collisions

Short-answer questions

1 State one possible parameter for increasing the rate of each of the following reactions. Choose a *different procedure* in each case.

a A 1 cm cube of zinc is added to 4.0 mol L^{-1} HCl.
b Hydrogen peroxide decomposes to water and oxygen.
c A large crystal of washing soda (hydrated sodium carbonate) is reacted with 1.0 mol L^{-1} nitric acid.
d Solutions of 0.1 mol L^{-1} of potassium iodide and lead (II) nitrate are mixed and a yellow precipitate of lead(II) iodide forms.

2 Examine the potential energy diagram for a chemical reaction.



a Determine ΔH and the activation energy for the forward reaction.

b State if the reverse reaction is exothermic or endothermic.

c When the forward reaction occurs, determine if the temperature of the surroundings increases or decreases.

d Predict how ΔH and the activation energy will be affected if a catalyst is added to the system.

e On the same axes, sketch the approximate potential energy diagram for the catalysed reaction.

3 **a** Explain this statement:

'Many solid catalysts are used in pellet form or as wire gauze or as nanoscale particles, rather than as a large sheet.'

b A reaction occurs according to the following equation:

$$X(g) + 3Y(g) \rightarrow 2Z(g)$$

i The rate of reaction of Y at a certain temperature is $2.4 \times 10^{-4}\,mol\,L^{-1}\,s^{-1}$. Calculate the rate of reaction of X at the same temperature.

ii The energy of activation for the forward reaction to produce Z as shown in the equation is $60\,kJ\,mol^{-1}$. The ΔH for the reaction as shown is $-90\,kJ\,mol^{-1}$. Calculate the energy of activation for the reverse reaction.

4 The activation energy for the decomposition of hydrogen peroxide to oxygen was measured in two separate experiments.

$$2H_2O_2(aq) \rightarrow 2H_2O(l) + O_2(g)$$

I The activation energy for the decomposition reaction when an enzyme was added was found to be $36.4\,kJ\,mol^{-1}$. The temperature of the reaction mixture increased.

II When platinum was added to another sample of the hydrogen peroxide solution, the activation energy was $49.0\,kJ\,mol^{-1}$. The temperature of the reaction mixture increased.

a State the function of the enzyme and platinum in each of these reactions.

b Sketch, on the same set of axes, the energy profiles for the decomposition of hydrogen peroxide with the enzyme and the decomposition using the platinum.

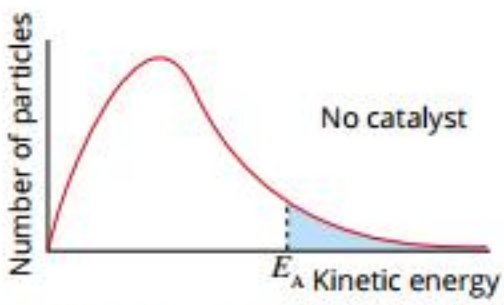
c Deduce which reaction system, I or II, would be faster. Explain your answer.

5 The enthalpy change for a particular reaction is $\Delta H = -26\,kJ\,mol^{-1}$

The activation energy for the uncatalysed reaction is $186\,kJ\,mol^{-1}$ and for a catalysed reaction it is $100\,kJ\,mol^{-1}$.

a On the graph below, sketch appropriately labelled energy profiles for both the catalysed and uncatalysed reactions.

b **i** The graph below illustrates the number of particles that decompose in a reaction system with no catalyst. Draw a graph to illustrate the reaction system if a catalyst were used.



ii Explain why a catalyst increases the rate of a reaction.

6 The fizzy sensation from sherbet lolly powder is caused by a gas produced in a reaction between two substances. The sherbet powder consists of the two dry reactants citric acid, $C_6H_8O_7$, and sodium hydrogencarbonate, and a sweetener such as icing sugar. The gas-producing chemical reaction does not begin until the dry ingredients become wet. As soon

as they dissolve into the saliva in your mouth, the reaction begins. In this reaction, the citric acid reacts with the hydrogencarbonate ions to form carbon dioxide (the fizz), water and citrate ions, $C_6H_5O_7^{3-}$.

a Explain in terms of the collision theory why a reaction occurs much quicker when the two reactants are 'wet'.

b Predict if you would expect the rate of 'fizz production' to change if some sherbet powder were to be poured into hot water. Explain your answer in terms of the collision theory.

7 Hydrogen gas is produced when a magnesium strip is added to dilute hydrochloric acid. The rate of reaction may change in any of these ways.

A The rate of reaction is decreased.

B The rate of reaction is increased.

C The rate of reaction is unchanged.

Choose the effect (A, B or C) that is most appropriate to each of the following situations. Justify your selection in terms of collision theory.

a The concentration of acid used is decreased.

b The reaction mixture is stirred.

c Magnesium in powdered form is used instead of a magnesium strip.

d The temperature is raised from 20°C to 30°C.

e A catalyst is added to the reaction mixture.

8 Ethanoic acid, CH_3COOH, is industrially manufactured from methanol according to the following reaction:

$$CH_3OH(l) + CO(g) \rightarrow CH_3COOH(l); \qquad \Delta H = -137\,kJ\,mol^{-1}$$

The most modern chemical plants now use rhodium, Rh, as a catalyst for this reaction.

a i Explain what is meant by the term '$\Delta H = -137\,kJ\,mol^{-1}$', written after the chemical equation.

ii Calculate the amount of heat released or absorbed when 100 g of ethanoic acid is formed in the reaction given above.

b i Explain the role of a catalyst in a reaction.

ii In terms of the collision theory, explain how a catalyst affects the rate of a reaction. Include an energy profile of the reaction in your answer.

9 When oxygen gas is reacted with hydrogen bromide, bromine gas is produced and heat is evolved according to the equation:

$$4HBr(g) + O_2(g) \rightarrow Br_2(g) + 2H_2O(g)$$

a Draw an energy profile for the reaction, clearly labelling the enthalpy of reactants and products, the ΔH for the reaction and the energy of activation. Indicate the parts on your diagram that represent the transition state, and the regions where energy is absorbed and released.

b i Define the term 'activation energy'.

ii Indicate how activation energy is related to the strength and number of bonds.

iii Describe the relationship between the rate of a reaction and activation energy

c Explain what is meant by the transitional state.

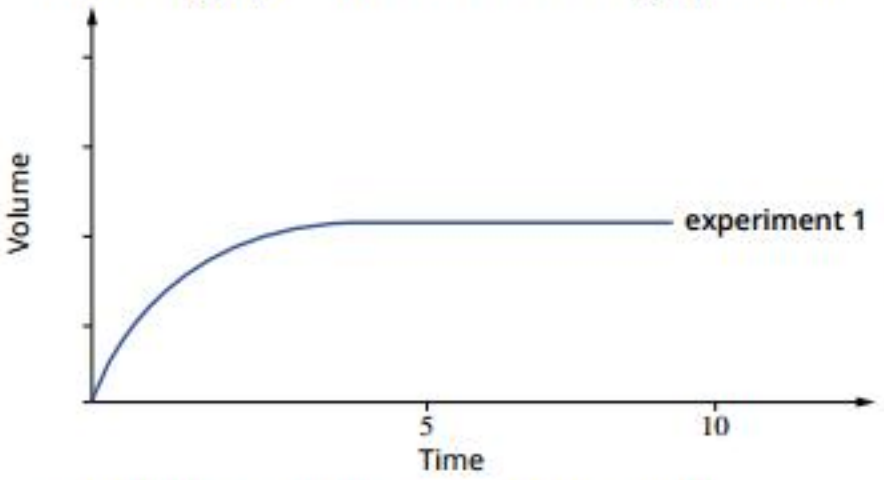
d The use of a catalyst does not change the value for ΔH for this reaction. Explain why.

e Express the rate of the reaction given above in terms of the rate of change in the concentration of reactants and products.

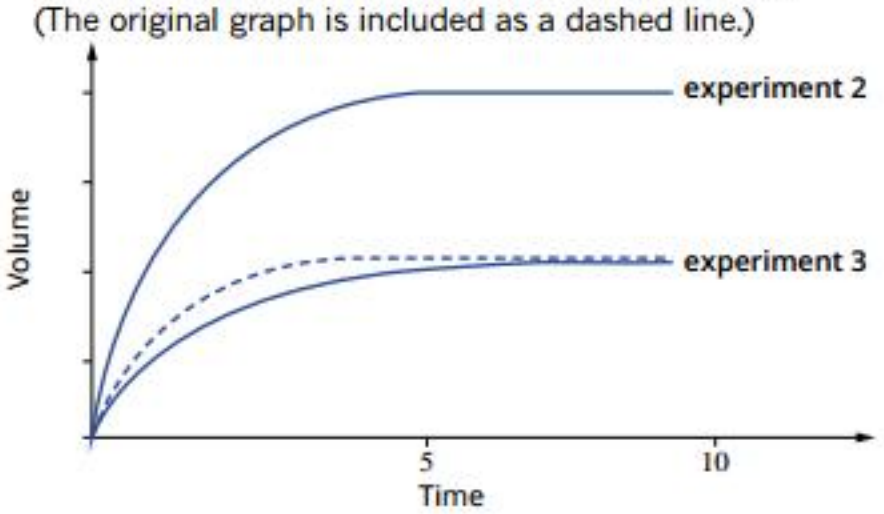
10 The equation for the reaction between magnesium and hydrochloric acid is:

$$Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$$

An experiment is conducted where 1.0 g of magnesium is added to excess hydrochloric acid at 25°C and the volume of hydrogen gas evolved is monitored. The volume of gas produced is shown on the graph below.



Two further experiments are conducted and the hydrogen gas evolved is shown on the graph below. (The original graph is included as a dashed line.)



a Suggest a change that was made to the original experiment that would have led to the hydrogen production as shown in experiment 2.

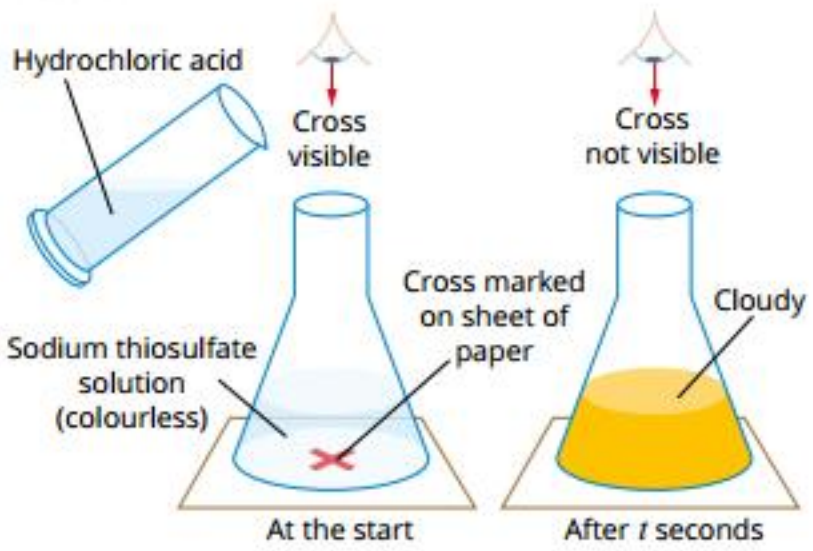
b Suggest three possible changes to experiment 1 that might have led to the hydrogen production as shown in experiment 3.

c List two other methods that could be used to monitor the rate of this reaction.

11 A student investigated the factors affecting the rate of reaction between a solution of sodium thiosulfate and hydrochloric acid. The equation for the reaction is:

$$Na_2S_2O_3(aq) + 2HCl(aq) \rightarrow 2NaCl(aq) + SO_2(g) + S(s) + H_2O(l)$$

The reaction was carried out in a conical flask placed on top of a piece of white paper with a dark cross marked on it. The rate of reaction was determined by measuring the time taken for the cross to be masked by the suspension of sulfur formed during the reaction, as shown.



The rate was determined for different concentrations of sodium thiosulfate and for different temperatures. The volume of each solution and the concentration of hydrochloric acid was kept constant. The results are summarised in the table below.

Experiment number	$[Na_2S_2O_3(aq)]$ (M)	Temperature (°C)	Time taken for the cross to be masked (s)
1	0.1	20	36
2	0.2	20	20
3	0.1	25	28

a Explain, in terms of collision theory, why the rate in experiment 2 is higher than the rate in experiment 1.

b Explain, in terms of collision theory, why the rate in experiment 3 is higher than the rate in experiment 1.

c Predict what factors, other than the two investigated in this experiment, may affect the rate of a reaction.

12 A group of students was asked to measure the rate of the reaction between 1.0 mol L^{-1} hydrochloric acid and marble chips (calcium carbonate).

a Write an equation for the reaction that occurs when marble chips are added to dilute hydrochloric acid.

Students investigated the rate of the reaction by measuring, at 10-second intervals, the volume of carbon dioxide collected in an inverted measuring cylinder (or gas syringe).

b Draw a labelled diagram indicating how you would assemble the apparatus.

The students' results are shown in the following table.

Time (sec)	Volume (mL)
0	0.0
10	27
20	44
30	54
40	60
50	65
60	68
70	71
80	73
90	74
100	76
110	77
120	78
130	79
140	80
150	80
160	80

c Draw a graph showing how the volume of carbon dioxide varies with time.

i How long does it take to collect 73 mL of gas?

ii Describe how you would determine the initial rate of reaction.

iii Determine the instantaneous rate at 10 seconds.

iv Calculate the average rate of production of carbon dioxide between 30 and 60 seconds.

v Calculate the average rate of consumption of hydrochloric acid between 30 and 60 seconds.

d Another student decided to determine the rate of the same reaction by recording the loss in mass in the reaction system at 10-second intervals.

i Explain why this would be a valid method for investigating the rate of the reaction.

ii Draw a labelled diagram indicating how the required apparatus could be assembled.

iii Draw a graph showing how the mass of the reaction system changes over time.

iv On the same graph, sketch the change in mass of the reactions system when the concentration of the hydrochloric acid used is 2.0 mol L^{-1} instead of 1.0 mol L^{-1}.

Practical manual

Practical investigations support the development of science inquiry skills and provide you with hands-on experience to deepen your understanding. The following science inquiry investigations offer opportunities for you to engage with practical applications of scientific concepts. These skills involve identifying and posing questions and working to answer them, evaluating claims, investigating ideas, solving problems, reasoning, drawing valid conclusions and developing evidence-based arguments.

Through these investigations, you will practice writing research questions, planning and conducting experiments, recording information, and reflecting on your processes. You will learn to process, analyse, and interpret evidence, evaluate conclusions and claims critically, and communicate your findings effectively.

Syllabus subject matter

Unit 1: Chemical fundamentals—structure, properties and reactions

Practical investigation 1—Investigate the empirical formula of a compound from reactions involving mass change

- Investigate the empirical formula of a compound from reactions involving mass change

Practical investigation 2—Investigate the enthalpy changes of a reaction

- Investigate the enthalpy change of a reaction, e.g. calorimetry or Hess's law.

Unit 2: Molecular interactions and reactions

Practical investigation 3—Investigate 3D molecular models

- Investigate 3D models of linear, bent, trigonal planar, tetrahedral and pyramidal molecules.*

  *Note: Simulations may be used.

Practical investigation 4—Investigate the molar volume of hydrogen gas

- Investigate Boyle's law or the molar volume of a gas

Practical investigation 5—Investigate precipitation reactions to identify cations and anions

- Investigate precipitation reactions to identify cations and anions

Practical investigation 6—Investigate factors affecting the rate of chemical reactions

- Investigate factors that affect the rate of chemical reactions

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Investigate the empirical formula of a compound from reactions involving mass change

Forming and finding

Aim

To investigate the research question: What is the empirical formula of magnesium oxide derived from reactions involving mass change?

Rationale (scientific background to the experiment)

By definition, a compound consists of elements chemically combined in fixed proportions by mass. When magnesium is heated in oxygen, the compound magnesium oxide forms. By finding the mass of the original magnesium and that of the magnesium oxide, using the law of conservation of mass, the mole ratio of magnesium to oxygen can be determined so that the empirical formula can be derived. The percentage composition of magnesium in magnesium oxide can also be calculated.

Timing

50 minutes

Materials

- magnesium ribbon 20–40 cm long
- steel wool
- crucible and lid
- pipeclay triangle
- Bunsen burner
- bench mat
- tripod
- tongs
- electronic balance
- safety glasses

PRE-LAB SAFETY INFORMATION

Material used	Hazard	Control
crucible	gets hot when heated	Use tongs to handle crucible when hot.
magnesium strips	creates a bright light when reacting with oxygen	Do not stare directly at magnesium when heating it.

Please indicate that you have understood the information in the safety table.

Name (print): _____

I understand the safety information (signature): _____

Method

Risk assessment

Consideration of risks include chemical and physical risks. Before you commence this practical investigation, you must conduct a risk assessment.

➤ Reflect and check the materials and method for risks

- ☐ Consider and account for risks/ethical issues/environmental issues in the materials and method.
- ☐ Conduct a risk assessment, completing the template in your Skills and Assessment book or downloading it from your eBook.

1. Your teacher will give you a 20–40 cm length of magnesium ribbon. Clean the magnesium ribbon thoroughly using steel wool.
2. Weigh the mass of a clean, dry crucible and lid. Place the magnesium loosely in the crucible. Weigh the total mass of crucible, lid and magnesium. Record your data in Table 1 on page 469.
3. Set up your experiment as shown in Figure 1.

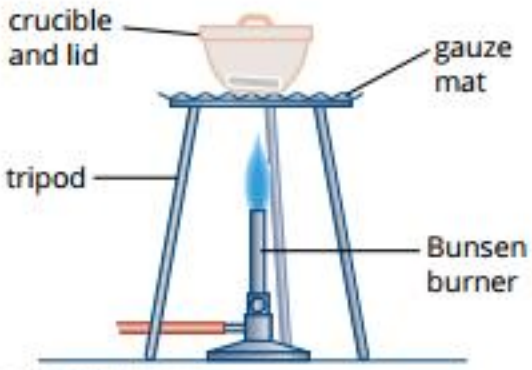


FIGURE 1 Experimental set-up

4 Heat the crucible strongly. Using tongs, occasionally lift the lid to allow air to enter the crucible but replace the lid quickly to avoid loss of magnesium oxide ash.

5 When the reaction appears complete, allow the equipment to cool to room temperature. Weigh the total mass of crucible, lid and magnesium oxide.

6 Calculate the original mass of magnesium used and the mass of magnesium oxide formed. Record the results in Table 1.

7 Assuming all the original magnesium is now in the form of magnesium oxide, calculate the percentage of magnesium in magnesium oxide. Record the result in Table 2. (Round off your result to the nearest per cent.)

8 Calculate:

- **a** the mass of oxygen that reacted with the magnesium
- **b** the number of moles of magnesium reacted
- **c** the number of moles of oxygen reacted
- **d** the simplest whole number mole ratio of magnesium to oxygen in magnesium oxide
- **e** the empirical formula of magnesium oxide

Variables

i Independent: the mass of magnesium
ii Dependent: the mass of magnesium oxide formed
iii Controlled: the crucible mass, the equipment and balance used

Analysing

Raw data

1 Record your data in Table 1.

TABLE 1 Mass results

Material	Mass (g)
empty crucible and lid (1)	
crucible, lid and magnesium (2)	
crucible, lid and magnesium oxide (3)	

Processed data

2 Calculate the mass of magnesium that reacted.

3 Calculate the mass of magnesium oxide that formed.

➤ Reflect and check that your data analysis demonstrates these characteristics

- ☐ Effective investigation of phenomena is demonstrated by the collection of sufficient and relevant raw data.
- ☐ Accurate application of algorithms, visual and graphical representations of data is demonstrated by appropriate processing and presentation of data to aid the analysis and interpretation of data.

Analysis

4 Calculate the percentage by mass of magnesium in magnesium oxide. Record your results in Table 2.

5 **a** Find out the result for percentage by mass obtained by three other groups that had different starting masses of magnesium. Record the results in Table 2.

TABLE 2 Group results

Group	Starting mass of magnesium (g)	Percentage by mass of magnesium (%)
your group		
other group 1		
other group 2		
other group 3		

b Explain why these results should be similar for each group, despite each group using a different mass of magnesium at the beginning of the experiment.

c If a group did not obtain a result similar to that of the other groups, suggest a reason for this occurring.

6 Calculate:

- **a** the number of moles of magnesium that reacted
- **b** the mass of oxygen, in grams, in your sample of magnesium oxide
- **c** the number of moles of oxygen that reacted
- **d** the ratio of moles of magnesium and oxygen

7 Using the result you obtained in Question **6d**, derive the empirical formula of magnesium oxide.

8 Determine how many atoms of magnesium were actually involved in your reaction. Use Avogadro's number to determine this.

9 **a** List each piece of equipment used in this experiment that had error associated with it. State the error value associated with each.

b Explain how this value may have had an effect on the determination of the empirical formula of magnesium oxide.

10 a Collect and process the data from your experiment and the results of three other groups. What is the most scientifically appropriate way to display the comparison between the initial mass of the magnesium used and the four mole ratios of magnesium : oxygen that were obtained, so that a clear and valid trend can be seen?

b Create this display and explain what you observe.

c Assess if there are any points that do not fit the trend. Explain why this might be so.

➤ Reflect and check that your analysis demonstrates these characteristics

- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough and appropriate error analysis.
- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough identification of relevant trends, patterns and relationships.
- ☐ Insightful and valid interpretation of evidence is demonstrated by drawing a valid and defensible conclusion based on the analysis.

Interpreting and evaluating

Conclusion

1 a State your conclusion.

b State the evidence that you have collected that leads you to this conclusion.

Evaluation

2 a Considering your analysis and conclusion, decide if the experiment provided an effective and efficient method of determining the empirical formula of magnesium oxide.

b Judge if the level of uncertainty that you calculated in Analysis Question **9** was reasonable. (Provide values that were close to whole number ratios.)

Improvements

3 If you were to repeat the experiment, identify the steps that you would do differently. You should include these points in your answer.

a Explain how you would change the methodology and how this might improve the results.

b Consider how well you performed the tasks and the skills that you need to improve on in your technique.

c Explain how the collection of data could be improved or uncertainty reduced.

Extension

4 a Evaluate whether this methodology could be applied to determine the empirical formula of any metal oxide.

b Identify any limitations and possible problems that might restrict the use of this methodology to determine the empirical formula of other metal oxides.

➤ Reflect and check that your evaluation demonstrates these characteristics

- ☐ Critical evaluation of processes is demonstrated by a discussion of the reliability and validity of the experimental process supported by evidence such as the quality of the data (as quantified in the error analysis).
- ☐ Critical evaluation of the conclusion is demonstrated by a discussion of the veracity of the conclusions with respect to the error analysis and limitations or sufficiency of the data.
- ☐ Insightful evaluation of processes and conclusions is demonstrated by a suggestion of improvements or extensions to the experiment which are logically derived from the analysis of the evidence.

Enhancement questions

5 The percentage by mass of aluminium in alumina (aluminium oxide) is 52.9%. Calculate the mass of aluminium that could theoretically be extracted from 800 tonnes of alumina.

6 A 10 g sample of a certain oxide of tellurium (Te) contains 8.0 g of tellurium. Find its empirical formula.

Investigate the enthalpy changes of a reaction

Forming and finding

Aim

To investigate the research question: What are the enthalpy changes of a reaction?

Rationale (scientific background to the experiment)

Calorimetry is a technique for measuring the energy change during a chemical reaction.

A calorimeter is often calibrated by passing an electric current through a heating coil in the instrument. The temperature of the calorimeter and its contents increases in proportion to the amount of energy supplied by the heating coil. The calibration factor (joules of energy required per degree Celsius of temperature increase) is determined by measuring the temperature increase that results from a measured energy input. The value of the calibration factor depends upon the characteristics of the particular calorimeter.

Once calibrated, the calorimeter can be used to measure enthalpy changes in chemical reactions. While bomb calorimeters are used to determine the energy content of food, solution calorimeters are used to determine energy changes for processes that occur in solution. Figure 1 summarises the steps involved in calorimetry calculations.

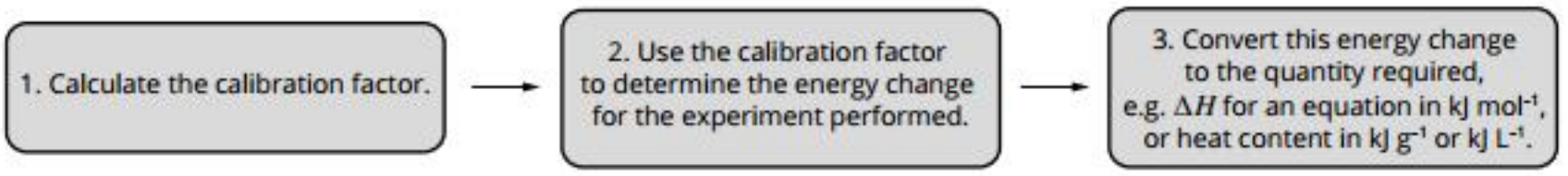

1. Calculate the calibration factor.
2. Use the calibration factor to determine the energy change for the experiment performed.
3. Convert this energy change to the quantity required, e.g. ΔH for an equation in kJ mol^{-1}, or heat content in kJ g^{-1} or kJ L^{-1}.

FIGURE 1 Steps involved in calorimetry calculations

Potassium nitrate is often used as a preservative in food and to help keep the colour of cured meats. In this experiment, you will determine the heat of solution when potassium nitrate dissolves in water.

Timing

50 minutes—can be split into two individual practicals, as long as students use the same calorimeter

Materials

- 100 mL measuring cylinder
- calorimeter (with a code number for identification)
- DC power supply
- 5 × wires leads
- thermometer, –10 to 50°C
- stopwatch
- ammeter
- voltmeter
- safety glasses
- 3 g potassium nitrate, coarsely ground
- spatula
- weighing bottle
- electronic balance

Method

Risk assessment

Consideration of risks includes chemical and physical risks. Before you commence this practical investigation, you must conduct a risk assessment.

➤ Reflect and check the materials and method for risks

- ☐ Consider and account for risks/ethical issues/environmental issues in the materials and method.
- ☐ Conduct a risk assessment, completing the template in your Skills and Assessment book or downloading it from your eBook.

PART A

1. Record the code number of your calorimeter in the space below Tables 1 and 2. You will need to use the same calorimeter after you have calibrated it.
2. Pour 100 mL of water into the calorimeter. Stir the water and record its temperature every 30 seconds in Table 1 for several minutes. (You could enter data directly into a computer spreadsheet program for later processing.)

PRE-LAB SAFETY INFORMATION		
Material used	**Hazard**	**Control**
use of electrical equipment	electric shock and damage to equipment	check all connections carefully
Please indicate that you have understood the information in the safety table. Name (print): _____ I understand the safety information (signature): _____		

3 Once the temperature is steady, apply a measured voltage of approximately 6V for exactly three minutes using the circuit shown in Figure 2. Stir continuously and record the temperature every 30 seconds.

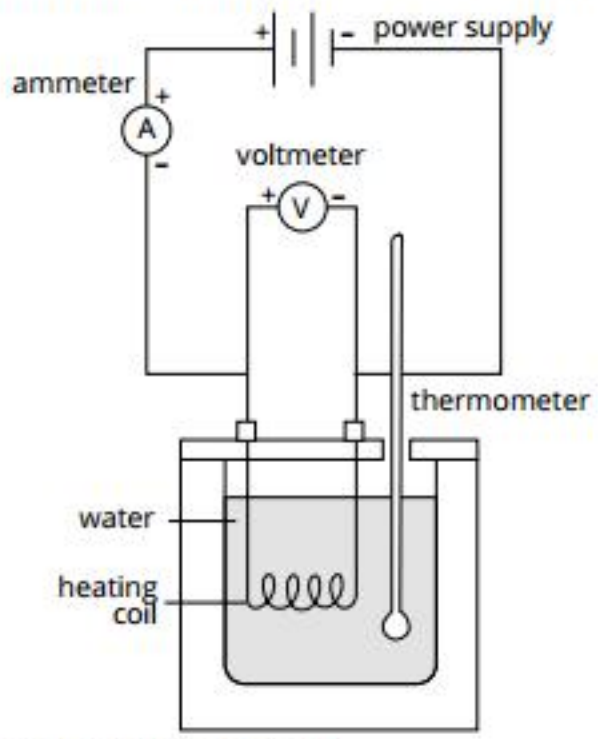


FIGURE 2 Experimental circuit set-up

4 Record the potential difference (voltage) and current while the water is heating. After three minutes, turn off the power supply. Continue to stir the water in the calorimeter and record its temperature every 30 seconds for a further three minutes.

5 Discard the water in the calorimeter and repeat steps 1–4 using a fresh supply of water. Record your results in Table 2 on page 473.

PART B

1 Pour 100mL of water into a calorimeter. Stir and record the temperature of the water.

2 Add about 3g of accurately weighed potassium nitrate to the calorimeter. Stir and record your results in Table 3 on page 473.

Variables

i Independent: the amount of potassium nitrate.

ii Dependent: the heat of solution when potassium nitrate dissolves in water.

iii Controlled: the calorimeter used, the balance used, the measuring cylinder used, the DC power supply, the ammeter and voltmeter, the thermometer used.

➤ Reflect and check that your evaluation demonstrates these characteristics

- ☐ Effective and efficient investigation of phenomena is directed by a concise and relevant research question.
- ☐ Accurate application of scientific concepts, theories, models and systems is demonstrated by a considered rationale for the experiment including scientific justification for the chosen modifications.
- ☐ Effective and efficient investigation of phenomena is demonstrated by a considered methodology that enables the collection of sufficient, relevant data that addresses the research question.
- ☐ Safe investigation of phenomena is ensured through the consideration and management of risks, and ethical or environmental issues.

Analysing

Raw data

TABLE 1 Results for calibration 1

Time (min)	Temperature (°C)	Time (min)	Temperature (°C)	Time (min)	Temperature (°C)

Code number of your calorimeter: _____

TABLE 2 Results for calibration 2

Time (min)	Temperature (°C)	Time (min)	Temperature (°C)	Time (min)	Temperature (°C)

Code number of your calorimeter: _____

Potential difference during heating for calibration 1: _____ V

Current during heating for calibration 1: _____ A

Potential difference during heating for calibration 2: _____ V

Current during heating for calibration 2: _____ A

TABLE 3 Dissolution of potassium nitrate results

Mass (g) of KNO_3	
Initial temperature (°C)	
Final temperature (°C)	

Processed data

➤ Reflect and check that your data analysis demonstrates these characteristics

- ☐ Effective investigation of phenomena is demonstrated by the collection of sufficient and relevant raw data.
- ☐ Accurate application of algorithms, visual and graphical representations of data are demonstrated by appropriate processing and presentation of data to aid the analysis and interpretation of data.

1 Graph the two sets of data you collected when calibrating the calorimeter, plotting temperature against time.

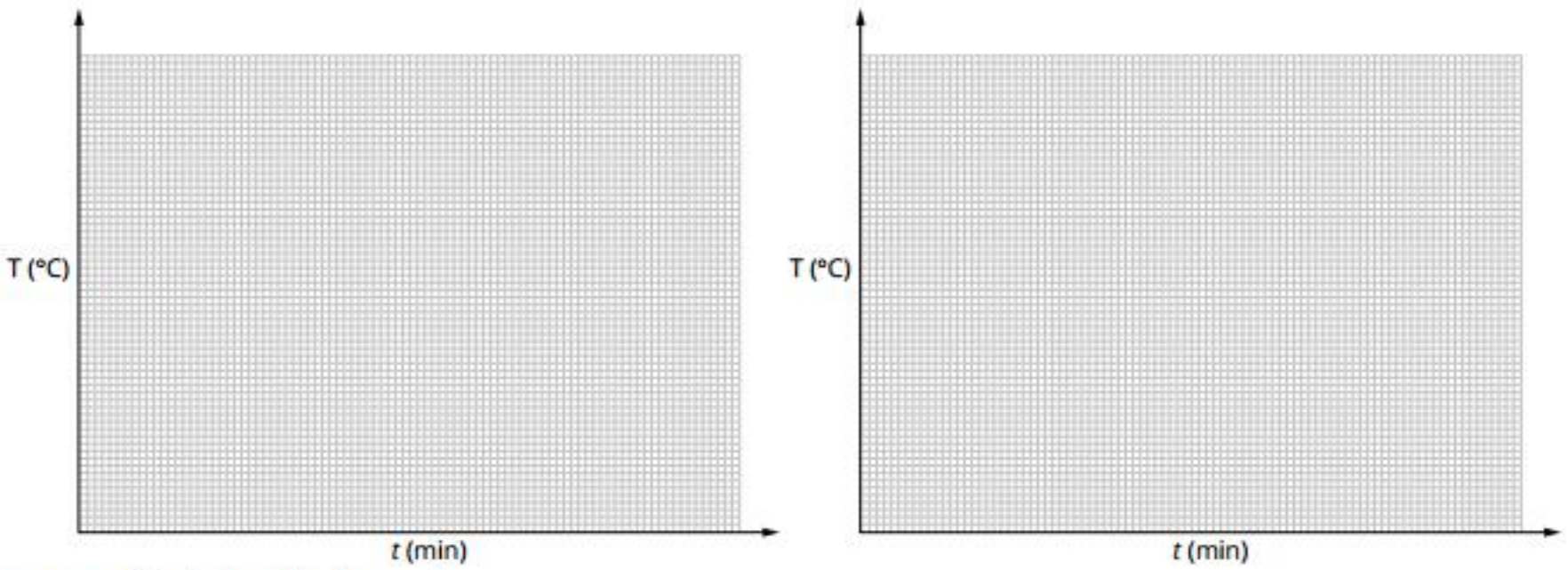


FIGURE 3 Calorimeter calibration graphs

2 For each set of data, record the calculations in Table 4.

TABLE 4 Data calculations

	First calibration	Second calibration
Temperature increase (°C) over the three minute heating period		
Thermal energy supplied by the heating coil in the calorimeter E = voltage (V) × current (amps) × time (s)		
Calibration factor for each set of data Calibration factor = $\frac{E}{\Delta T}$, where ΔT = temperature change (°C)		

Mean value of the two calibration factors: _____ $J\,°C^{-1}$

Analysis

➤ Reflect and check that your analysis demonstrates these characteristics

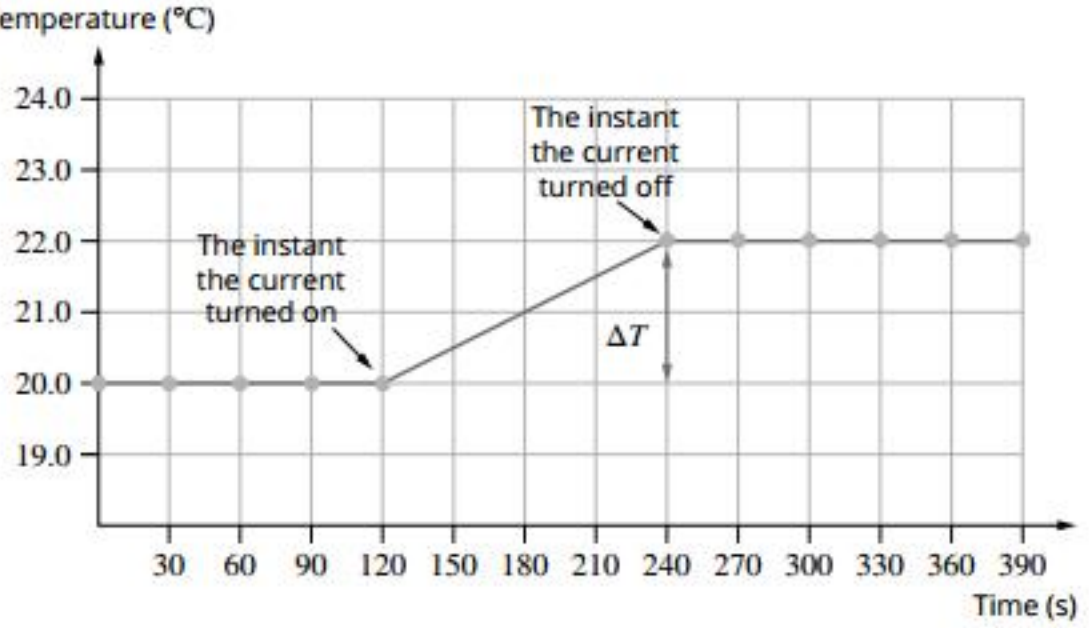
- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough and appropriate error analysis.
- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough identification of relevant trends, patterns and relationships.
- ☐ Insightful and valid interpretation of evidence is demonstrated by drawing a valid and defensible conclusion based on the analysis.

Discussion

1 What energy transformation occurs when the calorimeter and its contents are being heated?

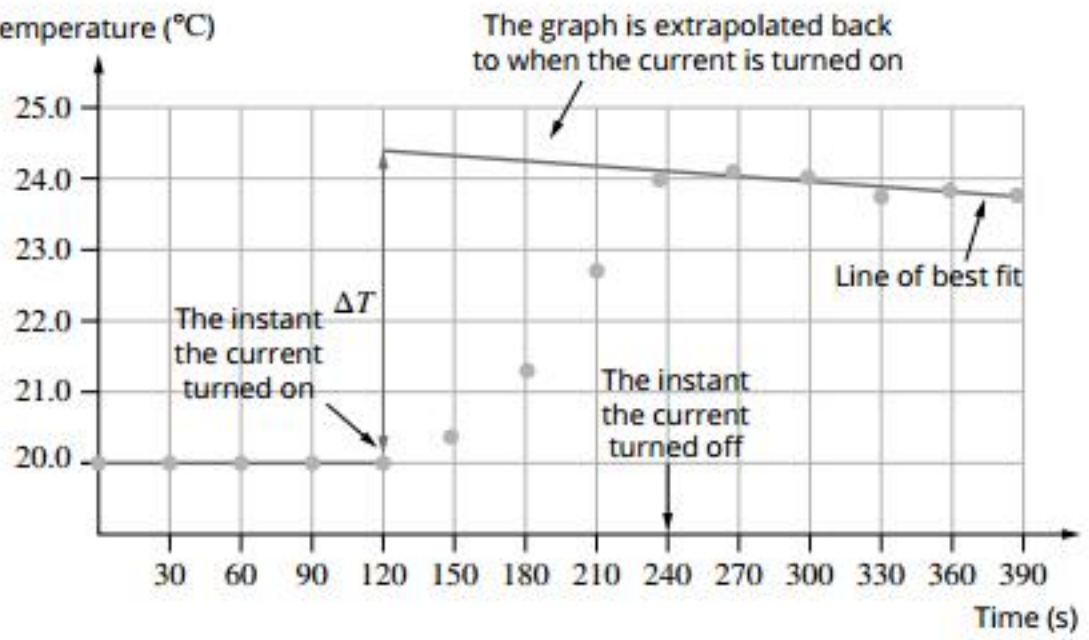
2 The graphs in Figure 4 show temperature against time for two calorimeters: (a) a graph for a well-insulated calorimeter and (b) a graph for a poorly insulated calorimeter with heat loss.
Compare these graphs to your graphs above.
Comment on the insulation of your own calorimeter.

a



Graph 1:
$\Delta T = T_{final} - T_{initial}$
$= 22.0 - 20.0$
$= 2.0°C$

b



Graph 2:
$\Delta T = T_{final} - T_{initial}$
$= 24.4 - 20.0$
$= 4.4°C$

FIGURE 4 Temperature–time graphs for the calibration of two calorimeters

3 What would be the effect on the calibration factor obtained from this experiment of using 50 mL of water instead of 100 mL of water to calibrate the calorimeter?

4 Write an equation for the dissolution of solid potassium nitrate in water.

5 Using your measurements of the changes in temperature and the calibration factor of the calorimeter, calculate the energy change, in joules, that occurred. (If the calibration factor is unknown, an estimate of the energy changed can still be calculated because 1 mL of water requires 4.18 J to raise the temperature by 1°C.)

6 Calculate the heat of reaction (ΔH) and give the sign for the ΔH.

7 For this reaction, which was the greater: the energy required to break the bonds in the reactants or the energy released when new bonds were formed to make the products? To explain your answer, draw an energy profile diagram and label it clearly.

8 Energy is neither created nor destroyed in a chemical reaction. Explain where the energy released (or absorbed) by the reaction comes from (or goes to).

Interpreting and evaluating

Conclusion

1 The experiment had the following aims.

a To calibrate a calorimeter. Based on your results were you able to determine a calibration factor for the calorimeter? What do your results suggest about the adequacy of your calorimeter?

b To determine the heat of solution when potassium nitrate dissolves in water. Based on your results, write a thermochemical equation for the reaction and state whether this was an exothermic or endothermic reaction.

Evaluation

2 Considering your analysis and conclusion, did the experiment provide an effective and efficient method of determining the heat of solution when potassium nitrate was dissolved in water?

3 How accurate do you think the results are based on the equipment used; that is, what percentage uncertainty do you expect? (Round to the nearest 10 per cent.)

Improvements

4 If you were to repeat the experiment, identify the steps that you would do differently. When considering this question you need to include in your answer issues with:

- the methodology and how you would change it to improve the results
- how you performed your tasks and the skills and whether you need to improve your technique
- the collection of data and how this could be improved or uncertainty reduced.

Extension

5 Suggest some practical improvements that could be made to the calorimeter you have calibrated and used to make your results more accurate.

6 Identify any limitations and possible problems that might restrict the use of this methodology in determining the heat of solution when a substance is dissolved in water.

➤ Reflect and check that your evaluation demonstrates these characteristics

- ☐ Critical evaluation of processes is demonstrated by a discussion of the reliability and validity of the experimental process supported by evidence such as the quality of the data (as quantified in the error analysis).
- ☐ Critical evaluation of the conclusion is demonstrated by a discussion of the veracity of the conclusions with respects to the error analysis and limitations or sufficiency of the data.
- ☐ Insightful evaluation of processes and conclusions is demonstrated by a suggestion of improvements or extensions to the experiment that are logically derived from the analysis of the evidence.

PRACTICAL INVESTIGATION 3

Investigate 3D molecular models

Forming and finding

Aim

To investigate the research question: How do 3D molecular models represent the bonding and shape of simple covalent molecules?

Rationale (scientific background to the experiment)

Making three-dimensional representations of covalent molecules provides a physical demonstration of the bonding and structure that is within a molecule. Models enable students to understand the concepts of molecular shape, symmetry, bond angles and polarity more clearly as they can rotate the structure and view it from different perspectives.

However, there are limitations to what these models can show, and, at all times while building these molecular models, students should be questioning what the differences are between the model and what they know of the actual molecule they are trying to represent.

Timing

60 minutes

Materials

- Commercially produced molecular model-building kit or lumps of different colours of plasticine and different length straws.
- If you are using straws or sticks to show bonds rather than a modelling kit, the lengths listed below should be used to represent the bonds of different types.

Bond type	Length of straw or stick (cm)
single covalent	5.0
double covalent	3.5
triple covalent	2.0
dispersion forces and hydrogen bonds	6.0

Method

Risk assessment

Consideration of risks includes chemical and physical risks. Before you commence this practical investigation, you must conduct a risk assessment.

➤ **Reflect and check the materials and method for risks**

- ☐ Consider and account for risks/ethical issues/environmental issues in the materials and method.
- ☐ Conduct a risk assessment, completing the template in your Skills and Assessment book or downloading it from your eBook.

1. Before building models of the molecules listed in Table 1, complete column two (Valence structure of the molecule to be built) and three (Lewis structure of the molecule to be built) of Table 1.
2. Using the appropriately coloured 'atoms', construct a model of each molecule listed in Table 1.
3. Draw each structure with a neat diagram that shows a three-dimensional representation of your model.
4. Repeat steps 1-3 for Table 2 then Table 3.

Analysing

Raw data

1. Record your results in Table 1, Table 2 and Table 3.

TABLE 1 Single covalent bonds

Molecule	Valence structure	Lewis structure	3D structure
methane (CH_4)			
ammonia (NH_3)			
water (H_2O)			

hydrogen chloride (HCl)			
phosphine (PH_3)			
butane (C_4H_{10})			

TABLE 2 Double covalent bonds

Molecule	Valence structure	Lewis structure	3D structure
oxygen (O_2)			
carbon dioxide (CO_2)			
ethene (C_2H_4)			
methanal (CH_2O)			

TABLE 3 Triple covalent bonds

Molecule	Valence structure	Lewis structure	3D structure
nitrogen (N_2)			
ethyne (C_2H_2)			

Processed data

2 Consider each molecular model. Complete Table 4 by identifying each molecule's shape, whether it is polar or non-polar and the type/s of intermolecular force you would expect to exist between molecules for each of these substances.

TABLE 4 Molecule shape, polarity and intermolecular force

Molecule	Shape	Polarity	Intermolecular force/s
methane (CH_4)			
ammonia (NH_3)			
water (H_2O)			
hydrogen chloride (HCl)			
phosphine (PH_3)			
butane (C_4H_{10})			
oxygen (O_2)			
carbon dioxide (CO_2)			
ethene (C_2H_4)			
methanal (CH_2O)			
nitrogen (N_2)			
ethyne (C_2H_2)			

➤ Reflect and check that your data analysis demonstrates these characteristics

- ☐ Effective investigation of phenomena is demonstrated by the collection of sufficient and relevant raw data.
- ☐ Accurate application of algorithms, visual and graphical representations of data is demonstrated by appropriate processing and presentation of data to aid the analysis and interpretation of data.

Analysis

3 Name the polar molecules that you have built and explain why they are polar.

4 State at least two limitations of the models you have built in how well they account for the properties of the compounds named in Question **3**.

5 Name one or more elements that can form stable single, double and triple bonds with its own atoms.

6 Name two elements whose atoms never form double bonds.

7 Explain why the bonding pairs in CH_4 are arranged in a tetrahedral shape.

➤ Reflect and check that your analysis demonstrates these characteristics

- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough and appropriate error analysis.
- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough identification of relevant trends, patterns and relationships.
- ☐ Insightful and valid interpretation of evidence is demonstrated by drawing a valid and defensible conclusion based on the analysis.

Interpreting and evaluating

Conclusion

1 **a** State your conclusion.
b Describe the evidence you have collected that leads you to this conclusion.

Evaluation

2 Considering your analysis and conclusion, evaluate whether the experiment provided an effective and efficient method of modelling the bonding and shape of various simple covalent molecules.

Improvements

3 If you were to repeat the experiment, identify the steps that you would do differently. You should include these points in your answer.
a Explain how you would change the methodology and how this might improve the results.
b Consider how well you performed the tasks and the skills that you need to improve on in your technique.
c Explain how the collection of data could be improved.

➤ Reflect and check that your evaluation demonstrates these characteristics

- ☐ Critical evaluation of processes is demonstrated by a discussion of the reliability and validity of the experimental process supported by evidence such as the quality of the data (as quantified in the error analysis).
- ☐ Critical evaluation of the conclusion is demonstrated by a discussion of the veracity of the conclusions with respect to the error analysis and limitations or sufficiency of the data.
- ☐ Insightful evaluation of processes and conclusions is demonstrated by a suggestion of improvements or extensions to the experiment, which are logically derived from the analysis of the evidence.

PRACTICAL INVESTIGATION 4

Investigate the molar volume of hydrogen gas

Forming and finding

Aim

To investigate the research question: What is the molar volume of hydrogen gas at standard temperature and pressure (STP)?

Rationale (scientific background to the experiment)

Gases are produced when fuels burn. An understanding of the behaviour of gases and gas laws allows us to calculate the volume of gaseous products and compare volumes of greenhouse gases released by different fuels.

In this experiment, you will determine the number of moles of hydrogen gas produced in a reaction. From measurements of the gas volume and pressure, the molar volume of hydrogen at standard temperature and pressure (STP) can be calculated.

Timing

40 minutes

Materials

- 20 mL 2 M HCl
- 4.5 to 5 cm length of magnesium ribbon that has a mass of no more than 0.08 g
- 100 mL gas syringe
- set of apparatus to clamp the syringe to a retort stand
- 250 mL conical flask
- one-hole stopper to fit conical flask
- 4 cm length of glass tubing to fit the one-hole stopper
- approx. 50 cm length of rubber tubing to connect the gas syringe to the glass tubing in the one-hole stopper
- 100 mL measuring cylinder
- electronic balance
- emery paper or steel wool for cleaning the magnesium ribbon
- safety glasses

PRE-LAB SAFETY INFORMATION		
Material used	**Hazard**	**Control**
2 M HCl	Toxic by all routes of exposure; lung irritation	Wear eye and skin protection
Please indicate that you have understood the information in the safety table. Name (print): _____ I understand the safety information (signature): _____		

Method

Risk assessment

Consideration of risks includes chemical and physical risks. Before you commence this practical investigation, you must conduct a risk assessment.

➤ Reflect and check the materials and method for risks

- ☐ Consider and account for risks/ethical issues/ environmental issues in the materials and method.
- ☐ Conduct a risk assessment, completing the template in your Skills and Assessment book or downloading it from your eBook.

1 Clamp the stoppered gas syringe to its retort stand and connect the conical flask and syringe using the rubber tubing as shown in Figure 1. Check that the equipment is secure.

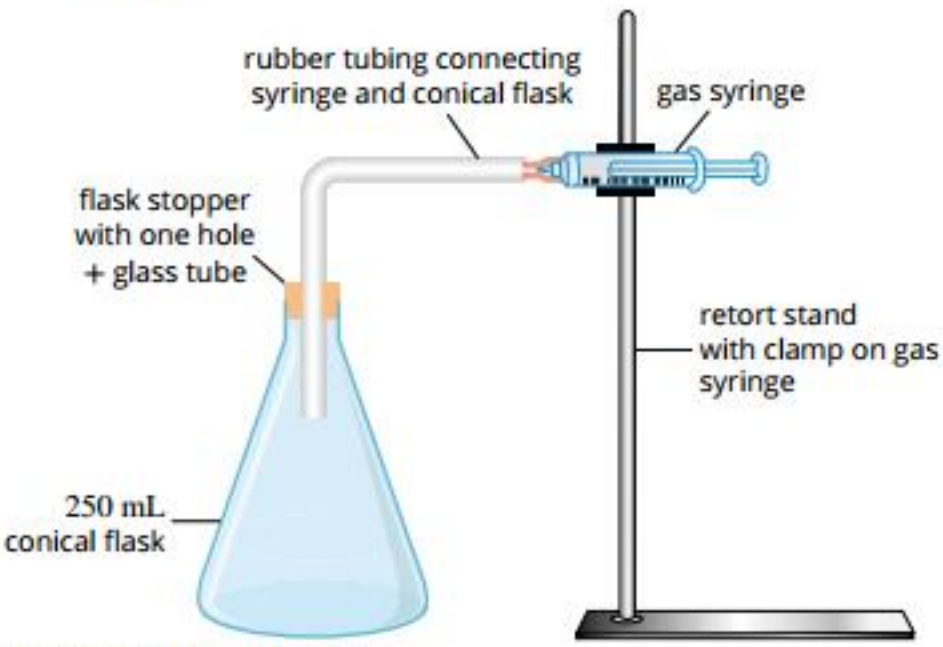

rubber tubing connecting syringe and conical flask
gas syringe
flask stopper with one hole + glass tube
retort stand with clamp on gas syringe
250 mL conical flask

FIGURE 1 Experimental set-up

2 Remove the stopper from the conical flask and carefully pour about 15 mL of 2 M hydrochloric acid into the flask without touching the sides.

3 Clean and accurately weigh the magnesium ribbon, making sure that it weighs no more than 0.08 g.

4 Tilt the flask and carefully place the magnesium ribbon on a dry side of the flask making sure that the magnesium does not contact the acid. Replace the stopper tightly, still keeping the flask tilted.

5 Carefully withdraw the plunger of the syringe and then release it. If the system has no leaks, the plunger will return to its original position. Once any leaks have been fixed, record the initial volume shown on the syringe in results Table 1.

6 Straighten the conical flask and shake the piece of magnesium into the acid. As gas fills the syringe, rotate the plunger gently to prevent it from sticking.

7 Once the magnesium has been used up, allow the conical flask to cool. In Table 1, record the final volume of gas in the syringe when the plunger has completely stopped moving. Calculate and record in the table the increase in the volume of gas in the syringe.

8 Record the room temperature and atmospheric pressure.

9 From data supplied by your teacher, record the water vapour pressure at room temperature. To allow for the pressure of water vapour in the syringe, subtract the water vapour pressure from atmospheric pressure.

Variables

i Independent: the mass of magnesium.

ii Dependent: the volume of hydrogen.

iii Controlled: the temperature, the atmospheric pressure, water vapour pressure at measured temperature.

Analysing

Raw data

1 Record your data in the table below.

TABLE 1 Experimental results

Results	
mass of magnesium (g)	
initial volume of syringe (mL)	
final volume of syringe (mL)	
volume of gas (mL)	
temperature (°C)	
atmospheric pressure, P_{atm} (kPa)	
water vapour pressure at measured temperature, P_{vapour} (kPa)	
pressure of H_2 gas = $P_{atm} - P_{vapour}$	

Processed data

2 Write a balanced equation for the reaction between magnesium and hydrochloric acid.

3 Calculate the amount, in mol, of magnesium reacted.

4 Using the amount of magnesium reacted, calculate the number of mol of H_2 produced.

➤ Reflect and check that your data analysis demonstrates these characteristics

- ☐ Effective investigation of phenomena is demonstrated by the collection of sufficient and relevant raw data.
- ☐ Accurate application of algorithms, visual and graphical representations of data is demonstrated by appropriate processing and presentation of data to aid the analysis and interpretation of data.

Analysis

5 The amount of H_2 gas occupied the measured volume at the experimental pressure and temperature. Calculate the volume occupied by one mole (molar volume) at these experimental conditions.

6 Convert your answer to Question **5** to molar volume at standard temperature and pressure conditions (STP), 0°C and 100 kPa.

7 How close is your result for the molar volume of hydrogen to the accepted molar volume of an ideal gas?

8 **a** List each piece of equipment used in this experiment that had error associated with it. State the error value associated with each.

b Explain how this value may have had an effect on the determination for the molar volume you have calculated.

9 Explain why the molar volume of any gas at specified conditions, such as STP, is the same.

10 Using your measurements for the volume, temperature and pressure of the hydrogen gas sample and the ideal gas equation, calculate the mole of H_2 gas produced. Compare your answer with your answer to Question **4**; how well do the two answers agree?

➤ Reflect and check that your analysis demonstrates these characteristics

- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough and appropriate error analysis.
- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough identification of relevant trends, patterns and relationships.
- ☐ Insightful and valid interpretation of evidence is demonstrated by drawing a valid and defensible conclusion based on the analysis.

Interpreting and evaluating

Conclusion

1 **a** State your conclusion.

b Describe evidence you have collected that leads you to this conclusion.

Evaluation

2 **a** Considering your analysis and conclusion, summarise whether the experiment provided an effective and efficient method of determining the molar volume of hydrogen.

b Describe whether the level of uncertainty that was calculated in Question **8** was reasonable. (Provide values that were close to whole number ratios.)

Improvements

3 If you were to repeat the experiment, identify the steps you would do differently. You should address these questions in your answer.

- **a** How would you change the methodology and how might this improve the results?
- **b** How well did you perform the tasks and are there skills that you need to improve on in your technique?
- **c** How could the collection of data be improved or uncertainty reduced?

➤ Reflect and check that your evaluation demonstrates these characteristics

- ☐ Critical evaluation of processes is demonstrated by a discussion of the reliability and validity of the experimental process supported by evidence such as the quality of the data (as quantified in the error analysis).
- ☐ Critical evaluation of the conclusion is demonstrated by a discussion of the veracity of the conclusions with respect to the error analysis and limitations or sufficiency of the data.
- ☐ Insightful evaluation of processes and conclusions is demonstrated by a suggestion of improvements or extensions to the experiment, which are logically derived from the analysis of the evidence.

Investigate precipitation reactions to identify cations and anions

Forming and finding

Aim

To investigate the research question: How can precipitation reactions be used to identify cations and anions?

Rationale (scientific background to the experiment)

An important aspect of chemistry involves qualitative analysis—the process of finding out what substances are present in an unknown sample. It is known as 'qualitative' because it is based on what substances are present, rather than on quantities that can be measured. This experiment uses the formation of a precipitate to identify unknown cations and anions.

For example, silver nitrate forms a white precipitate when added to any solution containing chloride ions, and therefore it is commonly used as a test for the presence of chloride ions.

Precipitation reactions are those that produce a solid when two solutions are mixed. The original reactants are soluble, but one of the products is insoluble, and precipitates out of solution. A precipitate generally forms very quickly, and may, in some cases, consist of fine particles. This gives the appearance of cloudy water or thick paint, depending on the nature and amount of precipitate formed. Some precipitates will slowly settle to the bottom of the test tube.

Timing

80 minutes

Materials

- dropping bottles containing the following test solutions:

Cations	Anions
Ba^{2+}	SO_4^{2-}
Al^{3+}	Br^-
Fe^{3+}	NO_3^-
Fe^{2+}	NH_3
Cu^{2+}	OH^-
Ca^{2+}	CO_3^{2-}
Pb^{2+}	I^-
Ag^+	Cl^-
Zn^{2+}	

- solutions of five unknown compounds, A to E
- semi-micro test tubes
- semi-micro test-tube rack
- safety glasses, lab coats

PRE-LAB SAFETY INFORMATION		
Material used	**Hazard**	**Control**
dissolved compounds of lead and barium	highly toxic by all routes of exposure; lung irritation	Wear eye and skin protection.
silver nitrate	can burn and stain skin and clothes	Wear eye and skin protection.
compounds containing Fe^{3+}, Cu^{2+} and I^-	can cause skin and eye irritation	Avoid contact, and wear eye and skin protection.
calcium hydroxide	slightly toxic if ingested	Wear eye and skin protection.
Please indicate that you have understood the information in the safety table. Name (print): _____ I understand the safety information (signature): _____		

Method

Risk assessment

Consideration of risks includes chemical and physical risks. Before you commence this practical investigation, you must conduct a risk assessment.

As directed by your teacher, complete the risk assessment and management table by referring to the hazard labels on the reagent bottles or safety data sheets (SDS) or your teacher's risk assessment for the investigation.

➤ Reflect and check the materials and method for risks

- ☐ Consider and account for risks/ethical issues/ environmental issues in the materials and method.
- ☐ Conduct a risk assessment, completing the template in your Skills and Assessment book or downloading it from your eBook.

Each of the unknown solutions A to E contains one dissolved ionic compound.

Table 1 gives a brief description of precipitates formed when various cations and anions are allowed to react. This information will assist you in identifying the cation and anion present in the ionic compound in solution. In some cases the distinctive colour of a precipitate formed will be sufficient to identify one of the ions in solution. In other cases, you may need a few tests to isolate the ion.

TABLE 1 Formation of precipitates

- White, green, yellow and so on means the precipitate is visible on the bottom of the test tube.
- Cloudy means the precipitate is uniformly suspended in the water.
- For blank spaces, the substance is assumed to be soluble, giving a clear (possibly coloured) solution.

Cations used to identify the anion ↓	**Anions used to identify the cation**							
	nitrate NO_3^-	sulfate SO_4^{2-}	carbonate CO_3^{2-}	chloride Cl^-	iodide I^-	bromide Br^-	hydroxide OH^-	hydroxide (OH^-) with ammonia (NH_3) added
sodium Na^+								
potassium K^+								
barium Ba^{2+}		white	white				cloudy	
calcium Ca^{2+}			cloudy white				cloudy	
aluminium Al^{3+}			cloudy				cloudy (light)	cloudy
zinc Zn^{2+}			cloudy				cloudy	
iron(II) Fe^{2+}			grey-green				green	light green
iron(III) Fe^{3+}							brown	brown
copper Cu^{2+}			light blue		mustard		blue	
lead Pb^{2+}		white	white	cloudy	yellow	cloudy	white	white
silver Ag^+			light brown	white	light yellow	cream	brown	

Perform these steps to identify the anion present in each of the dissolved unknown ionic compounds.

1. Place about 20 drops of a selected unknown solution in a semi-micro test tube.
2. Carefully add a few drops, drop-wise, of one of the test cation solutions to the test tube.
3. In Tables 2a–e for the cation test, record:
   - **a** your observations and comment on the colour, lightness/darkness and density of any precipitate formed
   - **b** possible anions that would give results consistent with your test.
4. Choose a second test cation that will help you decide which of the possible anions identified in step 3 is present in your unknown solution. Test a fresh sample of unknown solution with this second cation and record your results in Tables 2a–e for the cation tests.
5. If necessary, repeat step 4 until you have clearly identified your unknown anion.
6. To identify the cation present in each of the unknown dissolved ionic compounds, repeat steps 1–5 using test anion solutions and putting your results in Tables 3a to 3e for the anion tests.
7. Deduce the formula of the ionic compound dissolved in each of the unknown solutions.

Variables

i. Independent: the anion or cation tested.

ii. Dependent: the colour change of solution and presence/absence of a precipitate.

iii. Controlled: the unknown substance tested, concentration of all substances.

Analysing

Raw data

1 Record your data for each of the unknown cation solutions A–E in Tables 2a to 2e.

TABLE 2A Cation test for unknown solution A

	Test 1	Test 2	Test 3	Test 4
Cation tested				
Observations				
Possible anions				

Anion for unknown solution A _____

TABLE 2B Cation test for unknown solution B

	Test 1	Test 2	Test 3	Test 4
Cation tested				
Observations				
Possible anions				

Anion for unknown solution B _____

TABLE 2C Cation test for unknown solution C

	Test 1	Test 2	Test 3	Test 4
Cation tested				
Observations				
Possible anions				

Anion for unknown solution C _____

TABLE 2D Cation test for unknown solution D

	Test 1	Test 2	Test 3	Test 4
Cation tested				
Observations				
Possible anions				

Anion for unknown solution D _____

TABLE 2E Cation test for unknown solution E

	Test 1	Test 2	Test 3	Test 4
Cation tested				
Observations				
Possible anions				

Anion for unknown solution E _____

2 Record your data for each of the unknown anion solutions A–E in Tables 3a to 3e.

TABLE 3A Anion test for unknown solution A

	Test 1	Test 2	Test 3	Test 4
Anion tested				
Observations				
Possible cations				

Cation for unknown solution A _____

TABLE 3B Anion test for unknown solution B

	Test 1	Test 2	Test 3	Test 4
Anion tested				
Observations				
Possible cations				

Cation for unknown solution B _____

TABLE 3C Anion test for unknown solution C

	Test 1	Test 2	Test 3	Test 4
Anion tested				
Observations				
Possible cations				

Cation for unknown C _____

TABLE 3D Anion test for unknown solution D

	Test 1	Test 2	Test 3	Test 4
Anion tested				
Observations				
Possible cations				

Cation for unknown solution D _____

TABLE 3E Anion test for unknown solution E

	Test 1	Test 2	Test 3	Test 4
Anion tested				
Observations				
Possible cations				

Cation for unknown solution E _____

Processed data

3 Identify each of the unknown solutions and write its formula.

4 Write an ionic equation for each reaction that led to the formation of a precipitate.

➤ **Reflect and check that your data analysis demonstrates these characteristics.**

- ☐ Effective investigation of phenomena is demonstrated by the collection of sufficient and relevant raw data.
- ☐ Accurate application of algorithms, visual and graphical representations of data is demonstrated by appropriate processing and presentation of data to aid the analysis and interpretation of data.

Analysis

5 A solution was thought to contain either copper ions or lead ions. Describe how you could identify which ions were present in the solution.

6 A solution was tested to determine the cation that was present, and the following results were obtained.

- The addition of dilute sulfuric acid (H_2SO_4) produced a white precipitate.
- The addition of dilute sodium hydroxide (NaOH) produced a white precipitate.
- The addition of potassium iodide produced a yellow precipitate.

Deduce the cation that was present.

7 A solution was thought to contain either Fe^{2+} or Fe^{3+} ions. Describe the minimum number of tests that could be conducted to identify the solution.

➤ **Reflect and check that your analysis demonstrates these characteristics.**

- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough and appropriate error analysis.
- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough identification of relevant trends, patterns and relationships.
- ☐ Insightful and valid interpretation of evidence is demonstrated by drawing a valid and defensible conclusion based on the analysis.

Interpreting and evaluating

Conclusion

1 **a** State your conclusion.

b What evidence have you collected that leads you to this conclusion?

Evaluation

2 Considering your analysis and conclusion, did the experiment provide an effective and efficient method of determining the positive and negative ions present in a series of unknown samples?

Improvements

3 If you were to repeat the experiment, identify the steps that you would do differently. You should include these points in your answer.

a how you would change the methodology and how this might improve the results

b how you performed the tasks and the skills that you need to improve on in your technique

c how the collection of data (identification of correct colours) could be improved

➤ **Reflect and check that your evaluation demonstrates these characteristics.**

- ☐ Critical evaluation of processes is demonstrated by a discussion of the reliability and validity of the experimental process supported by evidence such as the quality of the data (as quantified in the error analysis).
- ☐ Critical evaluation of the conclusion is demonstrated by a discussion of the veracity of the conclusions with respect to the error analysis and limitations or sufficiency of the data.
- ☐ Insightful evaluation of processes and conclusions is demonstrated by a suggestion of improvements or extensions to the experiment which are logically derived from the analysis of the evidence.

Investigate factors affecting the rate of chemical reactions

Forming and finding

Aim

To investigate the research question: How do changes in temperature and concentration of reactants affect the rate of a chemical reaction?

Rationale (scientific background to the experiment)

Hydrochloric acid reacts with sodium thiosulfate to produce sulfur, sulfur dioxide and water in the following reaction:

$$S_2O_3^{2-}(aq) + 2H^+(aq) \rightarrow S(s) + SO_2(g) + H_2O(l)$$

The sulfur precipitate causes the reaction mixture to become cloudy. The rate at which the solution becomes cloudy indicates the rate of reaction: the shorter the period before the cloudiness obscures a cross on a sheet of paper placed under the beaker, the more rapid the rate of reaction. In this practical investigation, the effects of temperature and concentration of one of the reactants on the rate of reaction are studied. Therefore, students should see an inverse relationship between the rate of reaction and time taken for the cross to disappear.

Timing

50 minutes

Materials

- 40 mL 2 M hydrochloric acid
- 100 mL 0.25 M sodium thiosulfate solution
- 10 mL measuring cylinder
- 100 mL measuring cylinder
- 6 × 100 mL beakers
- thermometer, –10 to 110°C
- Bunsen burner, tripod stand and gauze mat
- bench mat
- stopwatch
- black marking pen
- safety glasses

As directed by your teacher, complete the risk assessment and management table by referring to the hazard labels on the reagent bottles or safety data sheets (SDS) or your teacher's risk assessment for the investigation.

Method

Risk assessment

Consideration of risks includes chemical and physical risks. Before you commence this practical investigation, you must conduct a risk assessment.

➤ Reflect and check the materials and method for risks

- ☐ Consider and account for risks/ethical issues/ environmental issues in the materials and method.
- ☐ Conduct a risk assessment, completing the template in your Skills and Assessment book or downloading it from your eBook.

PART A: EFFECT OF TEMPERATURE

1. Mark a cross on a sheet of paper with a black marking pen.
2. Place a 100 mL beaker on top of the cross. Pour 10 mL of 0.25 M sodium thiosulfate solution and 35 mL of water into the beaker.
3. Record the temperature of the solution in Table 1 on page 488.
4. Add 5 mL of 2 M hydrochloric acid and commence timing. Measure and record in the table the time taken for the cross to disappear when viewed from above the beaker.
5. Pour 10 mL of 0.25 M sodium thiosulfate solution and 35 mL of water into another beaker. Heat the solution to approximately 40°C. Remove the beaker from the source of heat, place it on top of the cross, and immediately add 5 mL of hydrochloric acid. Again, measure and record the time taken for the cross to disappear.
6. Repeat step **5** with a third, fourth and fifth beaker, heating the solutions to approximately 50°C, 60°C and 70°C respectively.
7. Share your results with the class, to enable an average time to be determined for each temperature used.

PART B: EFFECT OF CONCENTRATION OF REACTANTS

1. Place a 100 mL beaker on top of a cross marked on a sheet of paper. Pour 10 mL of 0.25 M sodium thiosulfate solution and 35 mL of water into the beaker. Add 5 mL of 2 M hydrochloric acid and commence timing. Measure the time taken for the cross to disappear when viewed from above the beaker, and record this in Table 2 on page 488.

PRE-LAB SAFETY INFORMATION		
Material used	**Hazard**	**Control**
2 M HCl	toxic by all routes of exposure; lung irritation	Wear eye and skin protection.
Sulfur dioxide gas	toxic by inhalation; causes burns; risk of serious damage to the eyes	Avoid breathing gas; work in a well-ventilated area and dispose of reaction mixtures using a sink in a fume cupboard. Wear safety glasses.
Please indicate that you have understood the information in the safety table. Name (print): _____ I understand the safety information (signature): _____		

2 Place another 100 mL beaker on top of the cross. Pour 15 mL of the sodium thiosulfate solution and 30 mL of water into the beaker. Add 5 mL of hydrochloric acid and commence timing. Measure the time taken for the cross to disappear and record this in Table 2.

3 Place another 100 mL beaker on top of the cross. Pour 25 mL of the sodium thiosulfate solution and 20 mL of water into the beaker. Add 5 mL of hydrochloric acid and commence timing. Measure the time taken for the cross to disappear and record this in Table 2.

4 Place another 100 mL beaker on top of the cross. Pour 35 mL of the sodium thiosulfate solution and 10 mL of water into the beaker. Add 5 mL of hydrochloric acid and commence timing. Measure the time taken for the cross to disappear and record this in Table 2.

5 Place another 100 mL beaker on top of the cross. Pour 40 mL of the sodium thiosulfate solution and 5 mL of water into the beaker. Add 5 mL of hydrochloric acid and commence timing. Measure the time taken for the cross to disappear and record this in Table 2.

6 Share your results with the class to enable an average time to be calculated for the different concentrations of reactants used.

Variables

PART A: EFFECT OF TEMPERATURE

i Independent: the temperature of the solution.

ii Dependent: the rate of reaction as determined by the time taken for the cross to disappear.

iii Controlled: the volume and concentration of reactants, the size of the cross, the distance of viewing above the beaker, the person looking for the cross.

PART B: EFFECT OF CONCENTRATION OF REACTANTS

i Independent: the concentration of reactants by varying the volume of each used.

ii Dependent: the rate of reaction as determined by the time taken for the cross to disappear.

iii Controlled: the temperature, the size of the cross, the distance of viewing above the beaker, the person looking for the cross.

Analysing

Raw data

1 Record your data for each experiment.

TABLE 1 Experimental results for effect of temperature

Temperature (°C)	Time for the cross to disappear (s)

TABLE 2 Experimental results for effect of concentration of reactants

Solution	Concentration of sodium thiosulfate in solution (M)	Time for the cross to disappear (s)
10 mL $Na_2S_2O_3$ solution, 35 mL water and 5 mL HCl		
15 mL $Na_2S_2O_3$ solution, 30 mL water and 5 mL HCl		
25 mL $Na_2S_2O_3$ solution, 20 mL water and 5 mL HCl		
35 mL $Na_2S_2O_3$ solution, 10 mL water and 5 mL HCl		
40 mL $Na_2S_2O_3$ solution, 5 mL water and 5 mL HCl		

Processed data

2 Calculate the concentrations of the sodium thiosulfate in each of the reaction mixtures made up in Part B and enter those in the second column of Table 2.

3 Calculate the average time for the cross to disappear using all the class results for each temperature and each concentration. The class results tables should look similar to your results tables; however, the columns should read 'Average time for the cross to disappear (s)'.

➤ Reflect and check that your data analysis demonstrates these characteristics

- ☐ Effective investigation of phenomena is demonstrated by the collection of sufficient and relevant raw data.
- ☐ Accurate application of algorithms, visual and graphical representations of data is demonstrated by appropriate processing and presentation of data to aid the analysis and interpretation of data.

Analysis

4 Identify any differences between your group results and the class results for either of the tests. Deduce why this might have occurred.

5 After analysing the results, infer what effect an increase in temperature has on the rate of this reaction.

6 Conclude why an increase in temperature leads to a change in the rate of reaction.

7 After analysing the results, judge what effect increasing the concentration of sodium thiosulfate has on the rate of this reaction.

8 Explain why the rate of a reaction depends upon the concentration of the reactants.

➤ Reflect and check that your analysis demonstrates these characteristics

- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough and appropriate error analysis.
- ☐ Systematic and effective analysis of evidence is demonstrated by a thorough identification of relevant trends, patterns and relationships.
- ☐ Insightful and valid interpretation of evidence is demonstrated by drawing a valid and defensible conclusion based on the analysis.

Interpreting and evaluating

Conclusion

1 **a** State your conclusions. Ensure that you summarise the effects that a change in temperature and in the concentration of the reactants have on the rate of reaction.

b Identify the evidence that you have collected that leads you to make these conclusions.

Evaluation

2 Assess your analysis and conclusions. Judge whether the experiment provided an effective and efficient method of investigating the ways in which the changes in temperature and concentration of reactants affect the rate of a reaction.

Improvements

3 If you were to repeat the experiment, identify the steps that you would do differently. You should include these points in your answer.

a Explain how you would change the methodology and how this might improve the results.

b Consider how well you performed the tasks and the skills that you need to improve on in your technique.

c Explain how the collection of data could be improved or uncertainty reduced.

➤ Reflect and check that your evaluation demonstrates these characteristics

- ☐ Critical evaluation of processes is demonstrated by a discussion of the reliability and validity of the experimental process supported by evidence such as the quality of the data (as quantified in the error analysis).
- ☐ Critical evaluation of the conclusion is demonstrated by a discussion of the veracity of the conclusions with respect to the error analysis and limitations or sufficiency of the data.
- ☐ Insightful evaluation of processes and conclusions is demonstrated by a suggestion of improvements or extensions to the experiment that are logically derived from the analysis of the evidence.

Science as a human endeavour

Science as a human endeavour (SHE) features provide essential stimulus for the research investigation. These features are structured to develop foundational skills that support relevant science inquiry skills through the lens of Science as a human endeavour. This provides a suitable foundation from which students can launch into research investigation Internal Assessment 3 (IA 3) and build proficiency in Assessment Objectives 1, 2 and 3. Engaging with the SHE features will provide practice in writing research questions, planning and conducting experiments, recording information, and reflecting on their processes. They will learn to process, analyse and interpret evidence, evaluate conclusions and claims critically, and communicate their findings effectively.

Syllabus subject matter

Unit 1: Chemical fundamentals—structure, properties and reactions

Science as a human endeavour 1: Radioisotopes: nuclear medicine

- Appreciate that radioisotopes require careful evaluation and monitoring because of the potential harmful effects to humans and/or the environment.

Science as a human endeavour 2: Models of the atom: development of atomic theory

- Appreciate that experiments provided evidence that enabled scientists to develop models of the atom.

Science as a human endeavour 3: Distribution of elements in the universe

- Appreciate that analysis of the distribution of elements in living things, Earth and the universe has informed a wide range of scientific understandings.

Science as a human endeavour 4: Metallic nanoparticles

- Appreciate that the development of nanomaterials is important to meet a range of contemporary needs and have specific properties related to the size of the particles (1–100 nm).

Science as a human endeavour 5: Cellular respiration

- Appreciate that bodies rely on the exothermic reaction of respiration to provide us with sufficient energy.

Unit 2: Molecular interactions and reactions

Science as a human endeavour 6: Development of VSEPR theory

- Appreciate that two- and three-dimensional graphical models have been developed and adopted by chemists to represent and communicate the shapes of molecules.
- Consider the limitations associated with the VSEPR theory.

Science as a human endeavour 7: Decompression chambers

- Appreciate that safe scuba diving requires knowledge of the behaviour of gases.

Science as a human endeavour 8: Blood chemistry

- Appreciate that blood plasma is an aqueous solution containing a range of ionic and molecular substances.

Science as a human endeavour 9: Acid rain

- Appreciate that most sulfur dioxide released to the atmosphere comes from burning coal or oil in electric power stations.

Science as a human endeavour 10: Water quality

- Appreciate that knowledge of the composition of water from different sources informs decisions about how that water is treated and used.

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Radioisotopes: nuclear medicine

It is estimated that one-third to one-half of Australians will use radioisotopes and nuclear medicine for diagnosis or treatment of disease in their lifetime.

The use of these non-invasive chemicals in a way that targets a cell type or organ is increasing. Some radioisotopes are shown in Table 16.1.1. The usefulness of these isotopes for scanning and diagnostic purposes relies on the particles produced being detectable by imaging equipment, and having suitable half-lives to provide clear images while minimising radiation exposure. Additionally, the ability of these isotopes to selectively accumulate in specific tissues, cells or organs enhances their effectiveness in diagnosing and monitoring various medical conditions.

Conversely, radioisotopes used for radionucleotide therapy (RNT) should have a longer half-life and higher energy, and must be targeted to cells that need to be destroyed, such as tumour cells.

TABLE 16.1.1 Some common medical radioisotopes, their radiation emission type and half-life

Radioisotope	Radiation type	Half-life	Scan type
^{11}C	positron	20.4 minutes	PET—Alzheimer's, schizophrenia, depression
^{18}F	positron	110 minutes	PET—various brain and body scans
^{52}Fe	positron	8.3 hours	bone marrow scan
^{99}Tc	gamma	6 hours	bone, heart, brain scans
^{131}I	beta	8 days	thyroid imaging and radiotherapy
^{133}Xe	beta	5.3 days	lung function scan
^{177}Lu attached to a peptide	beta	160 days	radiotherapy—prostate cancer
^{192}Ir implant	gamma	94 days	radiotherapy—breast cancer
^{213}Bi attached to a specific antibody	alpha	45 minutes	radiotherapy—leukaemia, glioma, melanoma

Australia's only nuclear reactor at Lucas Heights, in south-west Sydney, is run by the Australian Nuclear Science Technology Organisation (ANSTO). It has increased the number of medical doses of radioisotopes produced from 550 000 in 2015 to many millions of doses to meet national and international demand. However, due to the very short half-life of some useful radioisotopes, these must be made in a cyclotron at a PET scanning facility (Figure 16.1.1). Only a few large hospitals in Australia have a cyclotron in their nuclear medicine department.

FIGURE 16.1.1 A cyclotron machine. The cyclotron is used to radioactively label chemicals for use in medicine. This is done by accelerating high energy particles and passing them through samples of the chemicals to be made radioactive.

The required radioactive properties determine whether a nuclear reactor or a cyclotron is used to produce a radioisotope.

- Atoms with extra protons in the nucleus are called neutron-deficient and are produced in a particle accelerator such as a cyclotron.
- Atoms with extra neutrons in the nucleus are called neutron-rich and are produced in a nuclear reactor.

Marie Curie, a Polish-born French physicist, made significant contributions to the study of radioactivity (Figure 16.1.2). She discovered the elements polonium and radium, using innovative techniques to isolate radioactive isotopes. Her groundbreaking work led to the world's first investigations into treating neoplasms with radioisotopes. Marie Curie's method of extracting radioisotopes posed risks due to her close and prolonged exposure to radioactive materials. She used her bare hands and lacked proper protective gear, which led to significant radiation exposure. This approach ultimately endangered her health and contributed to her untimely death from aplastic anaemia.

a

b

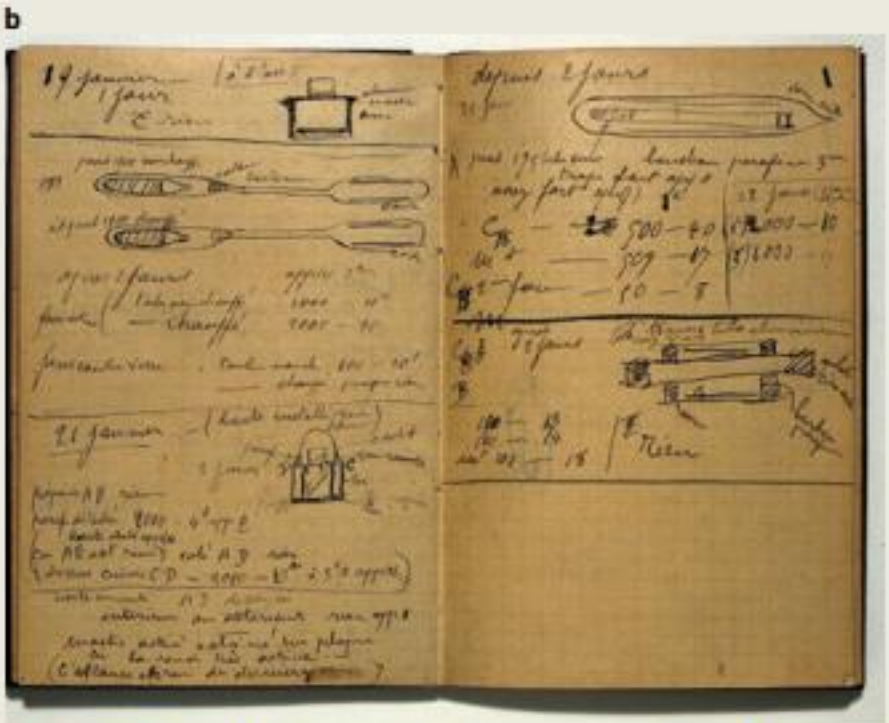


FIGURE 16.1.2 (a) Marie Curie and (b) her notebook, which still gives off radioactivity today and must be stored in a lead box for safety reasons.

Radioisotopes can be harmful to humans, as was the case with Marie Curie. As ionising radiation penetrates living matter, it gives up its energy through random interactions with atoms and molecules in its path, leading to the formation of reactive ions and free radicals. These biochemical changes can decrease the viability of cells or, more importantly, cause changes to DNA known as mutations. A change in the way a cell's growth is regulated may result in a cancer cell. Treatments involving high-energy radiation, and those where the radioisotope accumulates in a particular body tissue, are situations where cell damage can be expected. In the case of breast cancer treatment using ^{192}Ir (iridium), targeted cell death occurs when the radioisotope is implanted next to tumour cells.

Marie Curie's death significantly impacted safety protocols for working with radioisotopes. Her experience highlighted the need for rigorous protective measures, including shielding, time limits and distance from radioactive sources. Researchers and technicians now follow strict guidelines to minimise exposure and protect their health.

In practice, a variety of shielding structures are used, depending on the penetrating ability of the radiation. These may be as easy to use as a sheet of Perspex, or as cumbersome and heavy as a lead apron. Generally, scanning machines are automated to allow technicians to retire to an adjacent room or behind a barrier during the scan. It is vital that all recommended precautions are used, including daily monitoring of all surfaces used with a Geiger counter (an instrument that measures radiation levels). Personal radiation badges and monitors are checked daily or weekly. These have traditionally contained film, but thermoluminescent dosimeters (TLDs), aluminium oxide based dosimeters, and an electronic personal dosimeter (EPD) are increasingly being used. The safe use, storage and disposal of radioisotopes is outlined in the Code of Practice of the Australian Radiation Protection and Nuclear Safety Agency (ARPNSA). These procedures are put in place to protect patients and hospital staff.

Radionucleotides must be carefully handled to avoid contamination. Scientists, doctors and nurses must wear devices to monitor levels of radiation in their workplace. Three ways that this is done are shown in Figure 16.1.3.

FIGURE 16.1.3 Monitoring radiation in a nuclear medicine department takes many forms: (a) a Geiger counter, (b) a case film badge and (c) a radiation detector.

KEY QUESTIONS

Forming and finding

1 Identify two characteristics of a radioisotope suitable for medical imaging.

2 Research a common radioisotope from Table 16.1.1 on page 493 and describe how it acts to provide information or treat a disease.

3 Suggest two safety precautions that Marie Curie could have used that would have limited her exposure to radiation.

Analysing

4 Using Table 16.1.1 on page 493, can you identify patterns or trends in the data related to the methods of radiotherapy?

5 How might incorporating data from related studies enhance the validity of the research claim that radiotherapy implants are the best method for cancer treatment?

Models of the atom: development of atomic theory

The 30-year period at the start of the twentieth century saw scientists hypothesise, investigate, infer and confirm new understandings relating to the nature of the most fundamental particle of matter, the atom. Before that, at least 30 elements had been characterised, but little was known about the particles that comprised these substances. Laboratory equipment was basic and experimental data was used to make inferences about certain possibilities—this led to new experiments to unlock the mysteries of the atom. Between 1900 and 1935, one-third of the Nobel prizes in physics were awarded to researchers investigating the structure of the atom.

Dalton describes a basic particle of matter

Scientists investigating the structure of the atom used the insightful proposals made by John Dalton almost one hundred years earlier. In 1802, John Dalton presented the first **atomic theory of matter**. He meticulously measured the volumes of gases during reactions and observed them reacting in fixed ratios. Dalton proposed that all matter is made up of tiny spherical particles called atoms, which are indivisible and indestructible.

Dalton also accurately described elements as materials containing just one type of atom and compounds as materials containing different types of atoms in fixed ratios. Dalton's atomic theory of matter was mostly correct. Figure 16.2.1 is a copy of a page from Dalton's notebook showing his proposed system of denoting different elements as spheres, and a representation of his idea that these would form compounds by combining in predetermined ratios. As more elements were described, scientists decided to use the system of letters in use today.

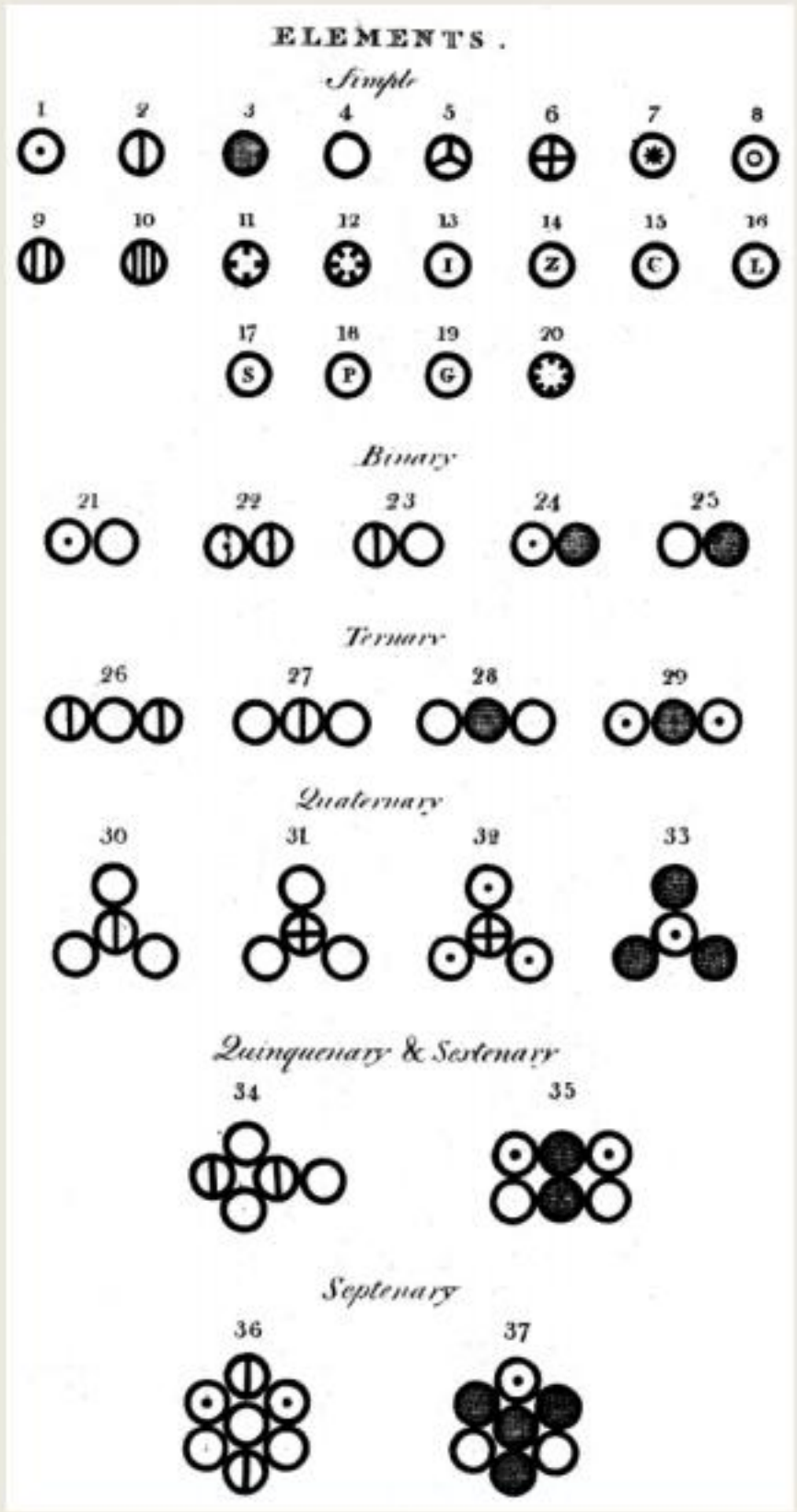


FIGURE 16.2.1 John Dalton's early system for identifying different elements

A negatively charged particle with very small mass

In the mid-nineteenth century, scientists could produce electric current. A series of experiments tested an electric current passed through different gases in sealed tubes (**cathode ray tubes**) at very low pressures. At high voltage, the cathode ray tubes glowed with a coloured light and the glass on the wall opposite the negative electrode became fluorescent (Figure 16.2.2).

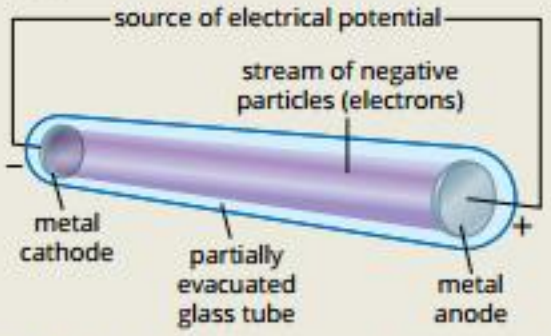


FIGURE 16.2.2 This glass cathode ray tube contains a gas at low pressure. When an electric potential is applied, a glow is observed on a phosphorescent screen. The particles responsible for the glow came from the cathode and travelled to the anode.

English physicist Joseph John Thomson repeated these experiments by using different metals as electrodes and different gases in the tube. In every case, the results were the same. The properties of the cathode rays were independent of both the gas and the metal. From his experiments in 1897, Thomson deduced that:

- the rays were a stream of particles with very low mass
- the particles came from the negative electrode (cathode) and were negatively charged
- the particles must be found in all matter and therefore were subatomic particles
- atoms must also contain positive subatomic particles since atoms have no overall charge.

Thomson proposed that the atom was a structure like a 'plum pudding' (Figure 16.2.3) with negatively charged particles throughout an area of positive charge. Thomson's research laid the foundation for other scientists to build the modern model of the atom. Importantly, excited physicists and chemists then began to investigate if there were smaller subatomic particles.

Robert A. Millikan was also fascinated by the nature of this negative charge. In 1910, he devised an experiment where the movement of charged oil droplets was changed by the voltage applied. He found that the charge on various-sized oil droplets was always a multiple of 1.5924×10^{-19} coulombs. His conclusion was that this was the charge on an electron.

FIGURE 16.2.3 After discovering a negative particle, Thomson proposed a 'plum pudding' structure of the atom that had negative particles distributed throughout a positive region.

An extremely dense body surrounded by empty space

Between 1899 and 1911, Ernest Rutherford conducted experiments in which he fired a beam of alpha particles at a piece of extremely thin gold foil. Most of the alpha particles passed straight through the gold foil. From this observation, Rutherford deduced that the gold atoms were made up almost entirely of empty space. Figure 16.2.4 shows the apparatus and observations of Rutherford's experiments.

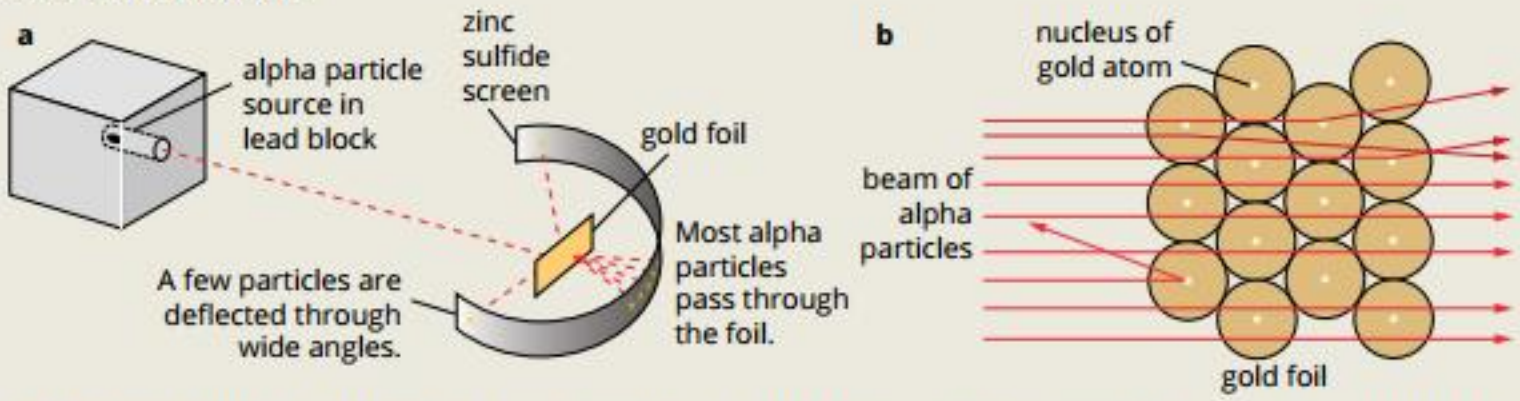


FIGURE 16.2.4 (a) Ernest Rutherford's apparatus that provided evidence for the discovery of nuclei in atoms. (b) Only those alpha particles that closely approach the nuclei in the gold foil were deflected significantly. Most particles passed almost directly through the foil.

However, Rutherford was surprised to discover that occasionally an alpha particle would bounce straight back. He stated: 'It was about as incredible as if you had fired a 16-inch shell at a piece of tissue paper and it came back and hit you!'

This remarkable observation suggested that the centre of the atom is very small, positive and extremely dense. This central region was later named the nucleus.

Rutherford provided experimental evidence for at least two subatomic particles (the proton and the electron). Rutherford's model (1911) proposed the following.

- Most of the mass of an atom and all of the positive charge is located in a tiny central region called the nucleus.
- Most of the volume of an atom is empty space, occupied only by electrons.
- The electrons move in circular orbits around the nucleus.
- The force of the attraction between the positive nucleus and the negative electrons is electrostatic.

Particles changing energy levels

Max Planck and Niels Bohr directed their research group to investigate energy-related phenomena. They wanted to explain why each element emits a characteristic spectrum of wavelengths of light. Bohr hypothesised that the best way to understand these emission spectra was to begin with the simplest element, hydrogen.

Bohr measured emission spectra of hydrogen first, followed by other elements. He found that the types of energy being emitted were specific to the element. In 1911, he proposed that this energy was the result of electrons moving between energy levels. This led to the shell model, which is the basis of the model in use today.

Later, in 1926, Erwin Schrödinger proposed that electrons behaved as waves around the nucleus. Using a mathematical approach and this wave theory, Schrödinger developed a model of the atom based on **quantum mechanics,** which describes how electrons exist in shells, subshells and orbitals.

Completion of a working model of the atom

As a working model for the atom began to emerge, scientists could still not explain why protons were not bursting out of the nucleus in every direction due to electrostatic repulsion.

In 1923, James Chadwick used a neutron chamber to collide alpha particles with boron or beryllium atoms. A type of radiation was produced that caused protons to be ejected from a sample of paraffin (Figure 16.2.5). Chadwick proposed that these heavy but uncharged particles, which he called neutrons, reside in the nucleus and that they bring stability to the nucleus by effectively shielding protons from each other.

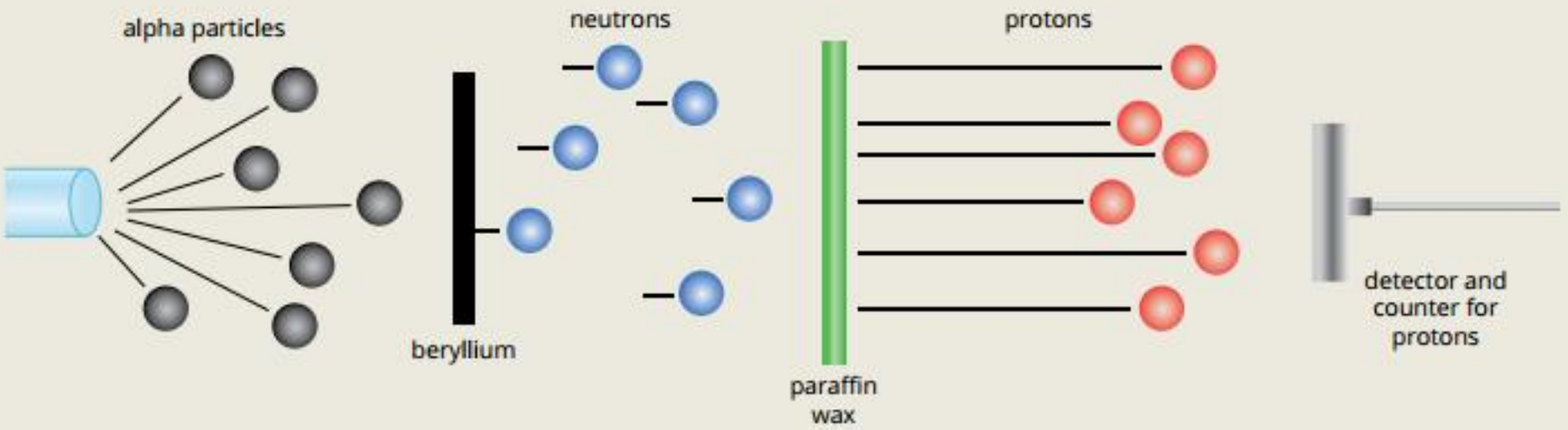


FIGURE 16.2.5 Schematic representation of the equipment used to identify the neutron. Alpha radiation pushes neutrons out of beryllium. The neutrons are heavy enough to force protons from a material such as paraffin wax.

Recent developments

Scientists of the twentieth century greatly enhanced our understanding of atomic structure (Figure 16.2.6).

It wasn't until 1981 that the scanning tunnelling microscope (STM), capable of viewing atoms, was developed by IBM researchers Gerd Binnig and Heinrich Rohrer. Using STMs, scientists confirmed that atoms are indeed spherical.

In the spirit of Rutherford and Chadwick, bombarding atoms with high-speed particles and other atoms continues to this day. These collisions can create new elements and allow characterisation of other subatomic particles. The **Large Hadron Collider** (LHC) has enhanced our understanding of ever smaller and more fundamental parts of the atom. Data produced in its massive 27 km underground 'atom smasher' supports the physicist's 'standard model' of subatomic particles. The most recent addition to this model is what some call the 'God' particle, the **Higgs boson**, confirmed in 2012. It is proposed that this particle is responsible for an atom demonstrating the measurable property of mass.

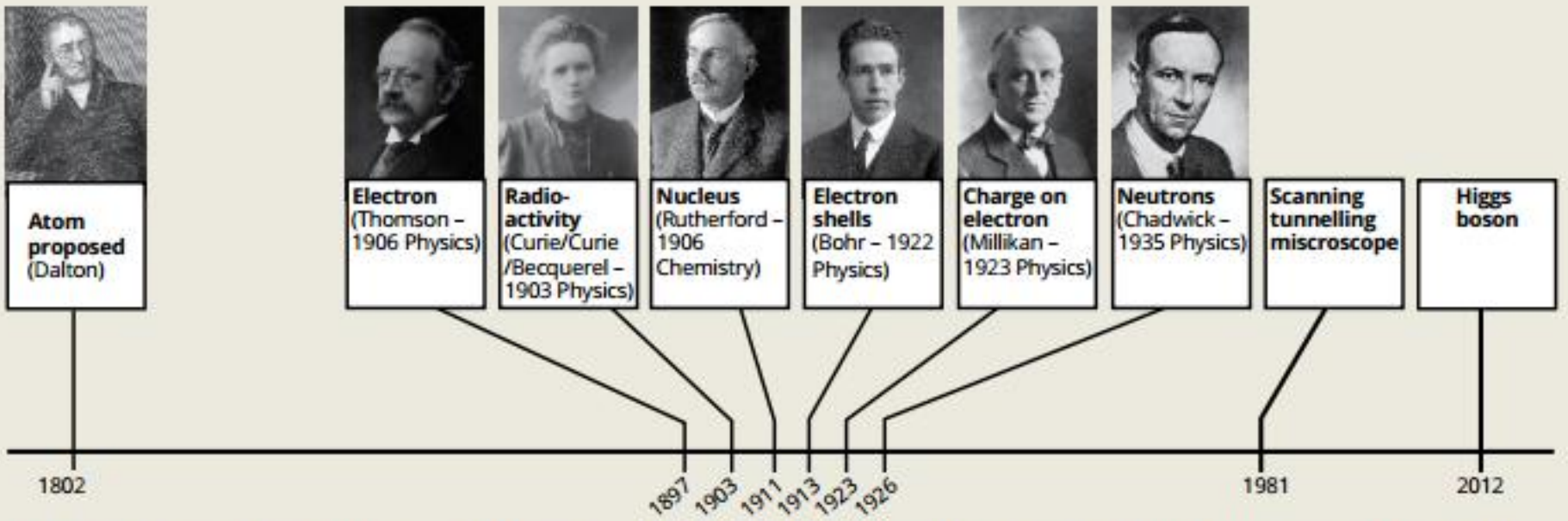


FIGURE 16.2.6 Timeline of key discoveries leading to our model of the atom. The scientist and year of their Nobel prize is shown in brackets.

KEY QUESTIONS

Forming and finding

1 Review Figure 16.2.4 on page 497 showing Rutherford's gold foil experiment. It showed that all the mass of the atom was in one place and that it was heavy enough to reflect alpha particles. Sketch the expected results of his experiment if Thomson's plum pudding model was correct.

2 Describe the finding of Millikan's oil drop experiment.

3 Explain the cathode ray tube experiment and the conclusions that Thomson developed during his investigations using this equipment.

4 In investigating phenomena, a scientist uses careful observation or experiments to report regularities or trends, known as laws. Subsequently, a scientific theory (a structure suggested by these laws) is devised to systematically explain them in a scientifically rational manner. Using two of the scientists described in this article, identify the law and the theory related to their experiments.

Analysing

5 Treat the experiments of Rutherford, Thomson and Chadwick as three pieces of evidence used to support an argument. What claim could they be addressing, and what is a possible research question for your claim?

6 What would be a limitation of one of these experiments?

Distribution of elements in the universe

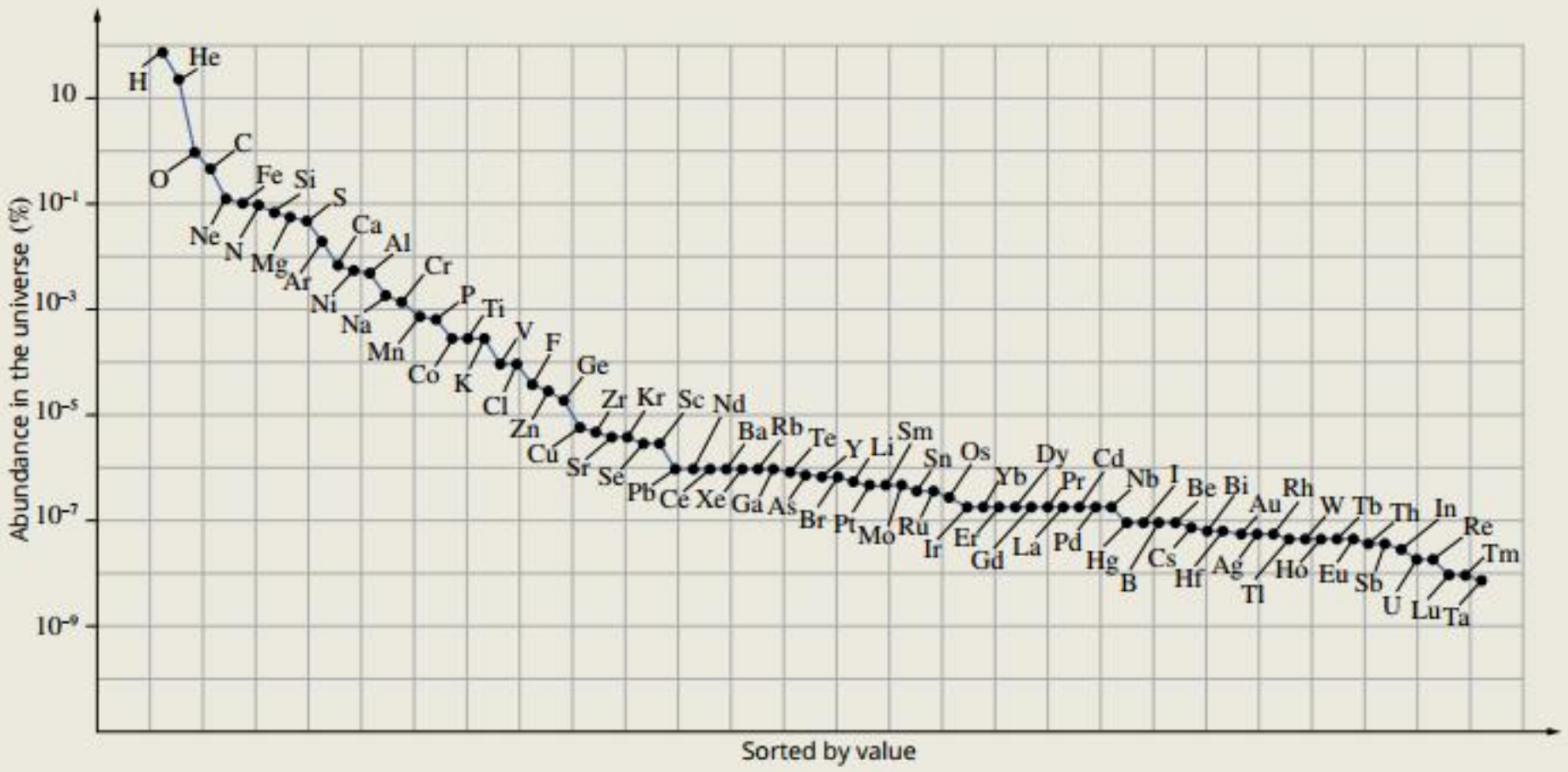

Abundance in the universe (%)
10
10⁻¹
10⁻³
10⁻⁵
10⁻⁷
10⁻⁹
Sorted by value
H He O C Ne N Fe Mg Si Ar S Ni Ca Na Al Mn Cr Co P K Ti Cl V Zn F Cu Ge Sr Zr Se Kr Pb Sc Ce Nd Xe Ba Ga Rb As Te Br Y Pt Li Mo Sm Ru Sn Ir Os Er Yb Gd Dy La Pr Pd Cd Hg Nb B I Cs Be Hf Bi Ag Au Tl Rh Ho W Eu Tb Sb Th U In Lu Re Ta Tm

FIGURE 16.3.1 Abundance of the elements in the universe

Scientists have discovered that matter in the universe is composed of about 100 elements. They propose that these elements have been formed by different nuclear reactions and that the distribution of elements within the universe reflects these processes and the relative nuclear stability of different nuclides.

Furthermore, cosmochemists have discovered that the distribution of elements within the universe (Figure 16.3.1) is very different from the composition of Earth. They conclude that this reflects the way Earth was formed and how organisms originated and evolved to what we have today.

There are several theories that have been proposed based on the analysis of the distribution of elements within living things, on Earth and in the universe.

Big Bang Nucleosynthesis (BBN)

While there is still much work to be done, analysis of the abundance of the elements indicates that the elements were formed following the Big Bang. The story of the BBN began in 1940 when Ralph Alpher performed theoretical calculations, which showed that the early universe contained neutrons. Some of these neutrons decayed into protons and electrons almost immediately as the universe expanded.

Alpher, Gamow and Bethe proposed that the nuclei produce heavier elements through the combination of additional nucleons. Their theory failed to predict the production of elements with more than five nucleons, since it relied on a stepping stone approach to the formation of elements.

It was 380 000 years after the Big Bang that the universe was sufficiently cool for the nuclei to capture electrons to form neutral atoms. Alpher and Robert Herman (Figure 16.3.2) predicted that this would emit cosmic microwave background (CMB) radiation, which was measured by Penzias and Wilson in 1964, confirming Alpher and Herman's theory.

FIGURE 16.3.2 From left to right, Robert Herman, George Gamow and Ralph Alpher

As the universe continued to expand and cool, the protons and neutrons captured the electrons to form the light elements, hydrogen (H) and helium (He), which make up to 99% of the mass of all elements in the universe. Fred Hoyle proposed that the fusion within stars is capable of forming the heavier elements, between carbon and iron.

Stellar evolution

Our universe is continuing to grow and expand. The spectral analysis of a star's light reveals its composition, temperature and motion. This analysis has revealed that stars are composed of elements up to iron (Fe) and that the universe is expanding.

Nuclear fusion reactions within stars allow the creation of elements up to iron (Fe), meaning that we are all small pieces of stars. Heavier elements than iron can't be formed through these nuclear fusion reactions and can only be formed through the massive forces involved in a supernova—the explosion of a star (Figure 16.3.3).

The fusion reactions that produce elements heavier than iron are endothermic and cause the star to lose energy. During the collapse of a star, the outer layers collide with the incompressible stellar core to produce a shockwave that expands outward through the unfused material of the outer shell. This induces fusion in that material, and the energy released leads to the star's explosion, dispersing material from the star into interstellar space.

FIGURE 16.3.3 The supernova remnant W49B. By tracing the distribution and amounts of different elements in the stellar debris field, researchers were able to compare the data gathered by the *Chandra* spacecraft to theoretical models of how a star explodes.

Dubbed the 'impossible' molecule, noble gases—such as helium, neon, argon, krypton, xenon and radon—typically refuse to form compounds due to their stable electron configuration. This refusal to form a molecule has meant that molecules containing noble gases don't occur naturally on Earth. However, astronomers have recently discovered noble gas molecules in space, challenging our understanding of these elusive elements. The Crab Nebula, a remnant of a massive star explosion, provided a unique laboratory for studying these compounds. From this investigation, it was assumed that in interstellar space, where extreme temperatures and densities are common, noble gases do things they would never do on Earth. That includes forming molecules.

Elements in our body

Despite its abundance in the universe, hydrogen makes up only 9% of our body. Ninety per cent of the elemental composition of our body comes from carbon (C), oxygen (O), nitrogen (N), sulfur (S) and phosphorus (P), with the remaining 1% from various trace elements.

One of these trace elements is calcium (Ca). When comparing the composition of humans to other life forms, elemental analysis shows that humans and bacteria are very similar. However, our use of calcium is very different. Humans contain approximately six times more calcium than bacteria, and bacteria actually excrete calcium. Calcium makes up bones, which give animals greater mobility.

KEY QUESTIONS

Forming and finding

1. Identify the key terms discussed in this article and define any that are new or that you are unfamiliar with in this context.
2. Identify key features of the formation of elements heavier than iron (Fe) within the universe.
3. Find one scientifically credible source, such as a podcast from the last six months or an article from a popular science website, that extends your knowledge on research being done on the 'impossible' molecule. Is this a primary or secondary source?

Analysing

4. Can you propose an explanation for the observed changes in the behaviour of noble gas molecules within the Crab Nebula based on the data analysis?
5. List some limitations that may be faced when gathering evidence on noble gas behaviours in the Crab Nebula.

Metallic nanoparticles

Nanomaterials have unique electrical, catalytic, magnetic, mechanical, thermal and imaging characteristics. This makes them attractive for use in medical, pharmaceutical, electronic and engineering sectors.

Gold nanoparticles in cancer treatment

Gold nanoparticles are the subject of substantial research, with a wide range of applications (Figure 16.4.1). One area of development is in using gold nanoparticles as a targeted chemotherapy treatment method.

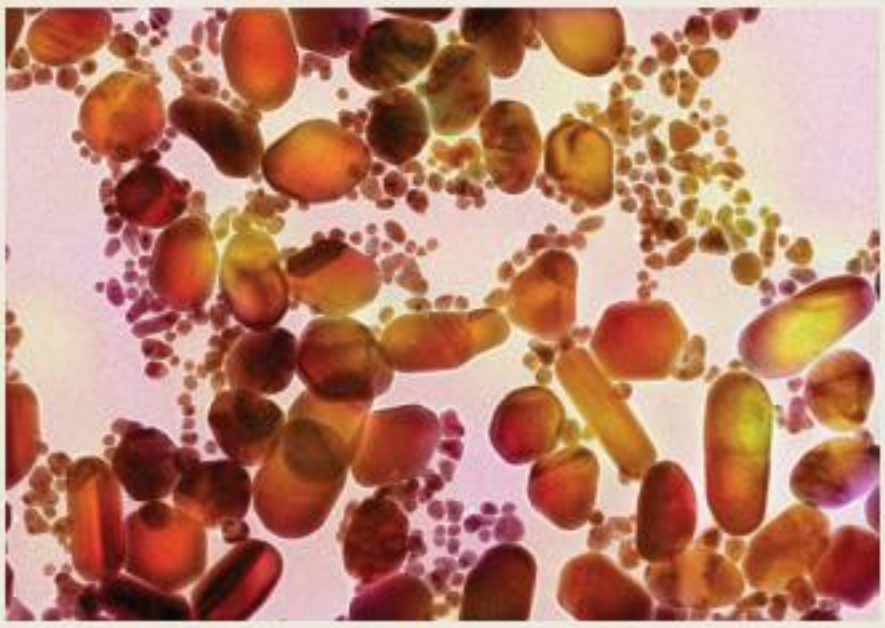


FIGURE 16.4.1 Applications of gold nanoparticles include cancer treatment research and detecting biological toxins.

Gold nanoparticles can be attached to molecules of a tumour-killing agent known as tumour necrosis factor (TNF). The nanoparticles hide the molecule from the body's immune system.

The nanoparticles carrying TNF tend to accumulate in cancer tumours, allowing TNF to destroy tumours. The nanoparticles do not appear to accumulate in other regions of the body, which means healthy cells are not affected.

Silver nanoparticles kill bacteria

Silver ions have long been known to kill bacteria. The ions can rapidly penetrate bacterial membranes and interact with proteins in the bacteria, destroying the cell structure of the bacteria and preventing them from reproducing.

Technology has enabled silver nanoparticles to be included in many different types of wound dressings. When the dressing (Figure 16.4.2) comes into contact with moisture from the wound, silver nanoparticles are slowly but continuously released from the wound pad. They then enter the wound and kill bacteria.

FIGURE 16.4.2 A wound dressing with silver nanoparticles to kill bacteria

In similar antibacterial applications, Samsung has created and marketed a material called Silver Nano, which adds silver nanoparticles to the surfaces of household appliances. Silver nanoparticles have been embedded in the surfaces of plastic storage bins, as well as in fabrics used by astronauts, babies and outdoor enthusiasts.

Copper nanoparticles go into space

Solder is a filler metal used to join two or more metals. Solders are essential to plumbing and metal constructions, including in satellites and spacecraft. For most of history, solders have contained a high amount of lead. Concerns about the toxicity of lead have driven the development of lead-free solder.

The complex electronics in satellites, such as the solar-powered satellite in Figure 16.4.3, must be reliable and efficient over a very long time. Space scientists have developed a nanotechnology copper-based solder that offers far superior performance over the materials currently in use. It is expected that the new solder material will produce up to 10 times the electrical and thermal conductivity of current solders, with a wide range of space and defence applications.

FIGURE 16.4.3 A nanotechnology copper-based solder has advantages in situations where long life and reliability are critical.

Iron nanoparticles remove pollution in groundwater

Iron nanoparticles are being used to clean up the pollutant carbon tetrachloride (CCl_4) from groundwater (Figure 16.4.4). Carbon tetrachloride is a manufactured toxic chemical that has been shown to cause cancer in animals. Spills of carbon tetrachloride can spread through soil and create large areas of contamination.

Iron nanoparticles can quickly and effectively break down carbon tetrachloride to a mixture of relatively harmless products. It may be possible to inject the nano-sized iron deep into the ground where it can treat contaminated groundwater.

FIGURE 16.4.4 Nanoparticles of iron are being investigated as a way of eliminating a range of environmental pollutants.

KEY QUESTIONS

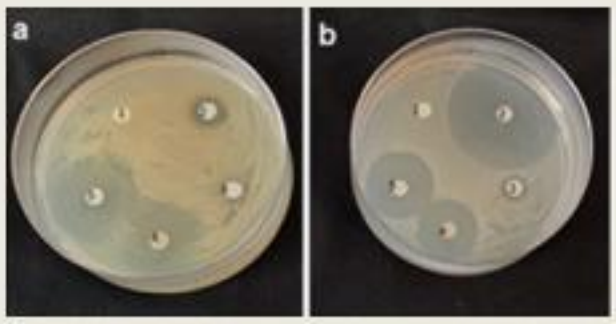
Forming and finding

1 Scientists at Swinburne University of Technology in Victoria have shown that gold nanorods can inhibit cancer cell growth in cervical cancer. Explain how the gold nanorods inhibit the cancer cell growth. Determine if this has been shown to affect all body cells.

2 Carbon tetrachloride (CCl_4) is a toxic chemical that has been used in fire extinguishers, as a coolant in refrigeration and as a solvent in dry cleaning. Spills of carbon tetrachloride can spread through the soil and create large areas of contamination. Explain how iron nanoparticles can be used to remove and break down this toxic CCl_4.

Analysing

A paper written by Smitha Chandrasekharan, Gandhimathi Chinnasamy and Somika Bhatnagar (2022) proposed sourcing silver nanoparticles through an eco-friendly approach known as phyto-fabrication. Phyto-fabrication uses logging residue, mainly the leaves, from trees (*Gmelina arborea*) to source the nanoparticles of silver (AgNP). Through experimentation, these AgNPs demonstrated excellent antibacterial properties against various pathogens, and also showed antioxidant activity and wound-healing potential (Figure 16.4.5).



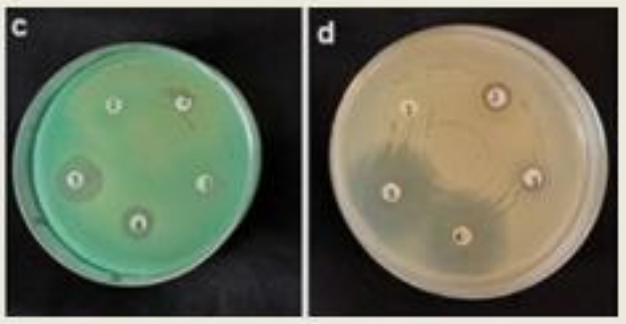


FIGURE 16.4.5 *Gmelina arborea (GA)*-sourced silver nanoparticles' antimicrobial effect on (a) *B. cereus*, (b) *E. coli*, (c) *P. aeruginosa* and (d) *S. aureus*. The treated numbers represent the control (1), the commonly used medical antibiotic Rifampicin (2), PF127 hydrogel (3), the GA-AgNPs (4) and the GA-AgNPs with the hydrogel (5).

3 What methods were employed to ensure the accuracy and reliability of the data analysis process?

4 What implications do the findings of the data analysis have for future research or practical applications in the field?

Cellular respiration

Living organisms are comprised of tiny membrane-bound compartments called cells. Most of the reactions that allow the cell to grow and function occur inside the cell. Cells contain, and are made up of, a diverse assortment of chemicals. These range from simple ions to highly complicated molecules, all in an aqueous solution known as the cytoplasm.

Metabolism refers to the chemical processes occurring within cells that are necessary for the maintenance of life. These chemical processes involve the breakdown of substances, usually the nutrients you obtain from food, to yield energy for vital processes. Another aspect of metabolism involves the synthesis of larger molecules such as proteins from smaller molecules. The breakdown and subsequent rebuilding of the nutrient molecules that are needed to sustain life involve condensation and hydrolysis reactions.

Complex molecules are formed through condensation reactions between simpler molecules. For example, starch is formed when simple glucose molecules react with each other, resulting in water molecules being formed (Figure 16.5.1). This is how cells assemble large and complicated molecules such as proteins and carbohydrates.

Hydrolysis reactions occur when water is added in the presence of a catalyst, such as an enzyme, to allow the breakdown of complex molecules into simpler ones. This is how cells break down complex carbohydrates into sugars, fats into fatty acids, and proteins into amino acids.

When foods such as carbohydrates are hydrolysed to the smaller glucose molecule, a redox reaction occurs in which O_2 reacts with the carbon and hydrogen atoms of glucose, forming oxides of carbon and hydrogen. The energy stored in the C–H and C–C bonds in glucose is released for the cell to use. This process is known as cellular respiration.

In cells that have a nucleus, respiration occurs on the inner membranes of cell organelles called mitochondria (Figure 16.5.2). The process is complex and involves dozens of intermediate reactions. This is because some of the bonds, in particular the C–C bond, do not oxidise easily. Also, energy must be released in a controlled way that does not damage the cell. Food molecules store considerable amounts of energy, and if they released their energy rapidly, as in combustion, the cell would likely be destroyed. Figure 16.5.3 is an enthalpy level diagram for the cellular respiration of sucrose, a type of simple carbohydrate molecule.

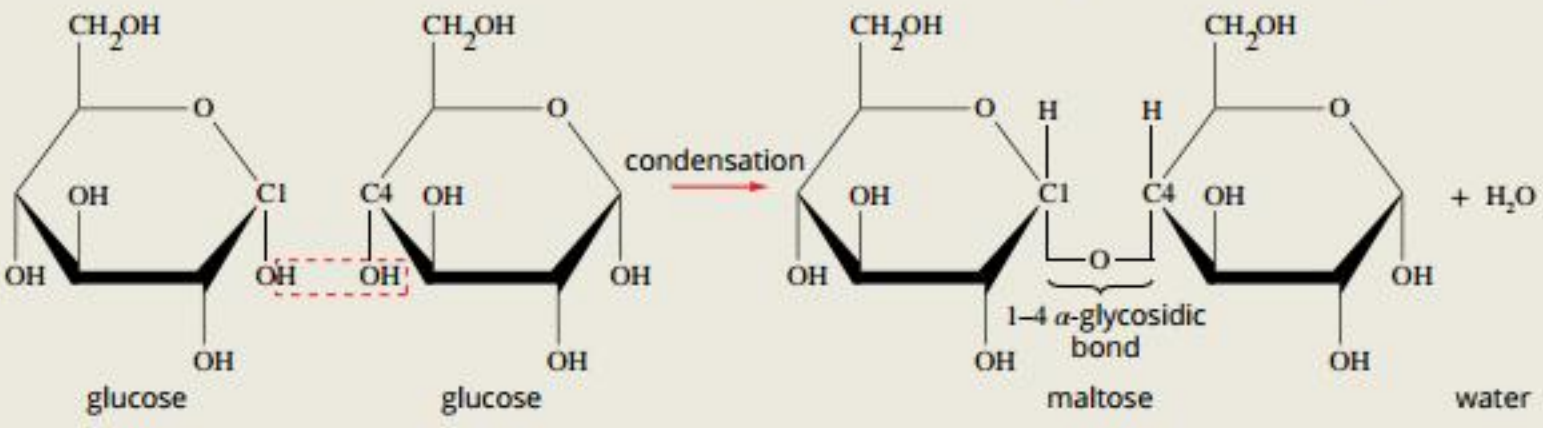


FIGURE 16.5.1 Condensation reaction between glucose molecules. Starch is formed when simple glucose molecules react.

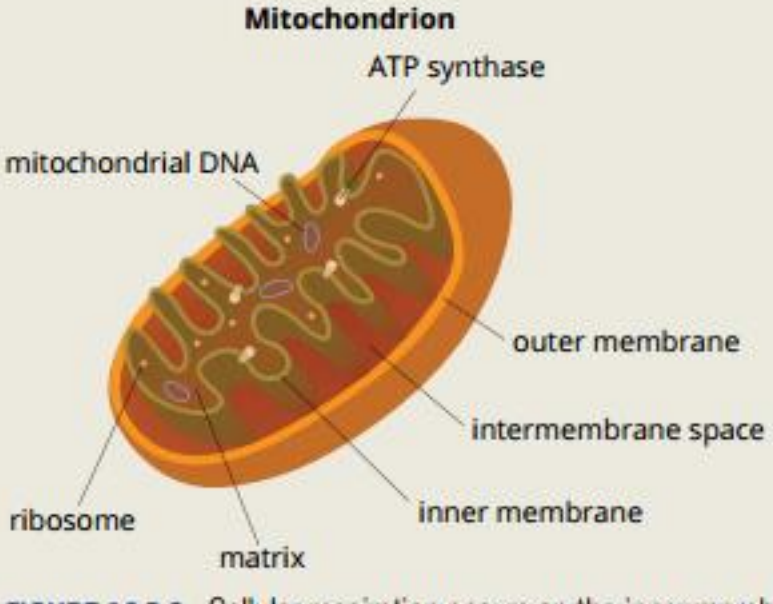


FIGURE 16.5.2 Cellular respiration occurs on the inner membranes of cell organelles known as mitochondria.

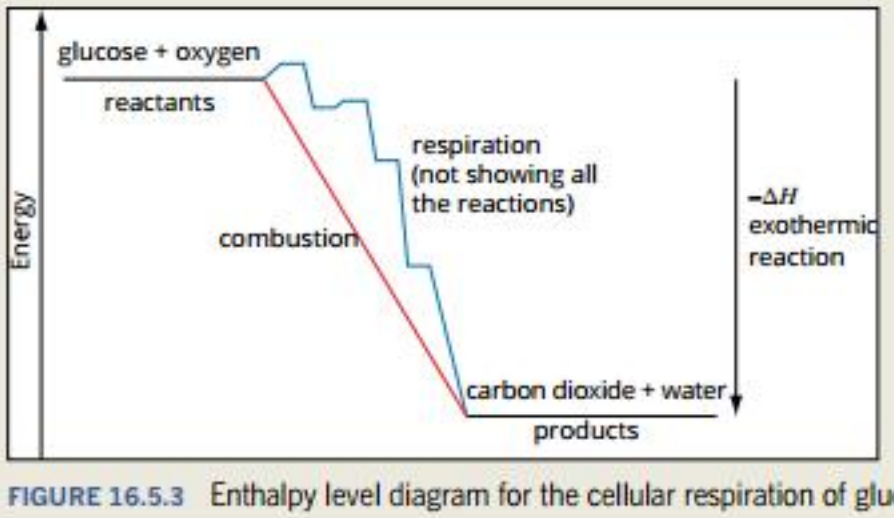


FIGURE 16.5.3 Enthalpy level diagram for the cellular respiration of glucose

There are two main types of cellular respiration.

- Aerobic respiration requires oxygen and is the main source of energy for the human body.
- Anaerobic respiration does not require oxygen and generally yields less energy.

In aerobic respiration, glucose is oxidised to carbon dioxide and water through a sequence of reactions. The overall equation for aerobic respiration is:

$C_6H_{12}O_6(aq) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$

$\Delta H = -2840\,kJ\,mol^{-1}$

In humans, an alternative form of respiration, called anaerobic respiration, can occur in muscles during prolonged and vigorous exercise, when the supply of oxygen is limited. It can result in the build-up of lactate ions, $CH_3CH(OH)COO^-$, which can cause painful muscular cramping (Figure 16.5.4). The overall equation for anaerobic respiration in humans is:

$C_6H_{12}O_6(aq) \rightarrow 2CH_3CH(OH)COO^-(aq) + 2H^+(aq)$

$\Delta H = -120\,kJ\,mol^{-1}$

FIGURE 16.5.4 The fatigue experienced by an athlete is partly due to formation of lactate ions produced by the anaerobic breakdown of glucose molecules in muscle cells.

In yeast, anaerobic respiration produces ethanol and carbon dioxide. This process, often referred to as fermentation, is used to produce alcoholic beverages. The equation for this process is:

$C_6H_{12}O_6(aq) \rightarrow 2C_2H_5OH(aq) + 2CO_2(g)$

$\Delta H = -69\,kJ\,mol^{-1}$

These reactions for anaerobic and aerobic respiration are all exothermic. Although anaerobic respiration yields less energy per mole of glucose, it is often a faster process than aerobic respiration. Short bursts of exercise, such as sprinting, rely on anaerobic processes for energy because the individual steps in the reactions involved in anaerobic respiration occur more rapidly.

KEY QUESTIONS

Forming and finding

1 Distinguish between hydrolysis and condensation reactions using carbohydrates as an example.

2 Determine whether cellular respiration is an endothermic or exothermic process.

3 Explain why cellular respiration involves dozens of intermediate steps.

4 Find one scientifically credible source, such as a podcast from the last six months or an article from a popular science website, that extends your knowledge on anaerobic respiration in yeast. List the reference, using appropriate referencing citations, and summarise the process of anaerobic respiration in yeast.

Analysing

5 Given that anaerobic respiration occurs within the cells of an organism, a student wondered how temperature would affect the rate of reaction. Design a controlled experiment to investigate the effect of temperature on the rate of anaerobic respiration in yeast. In your experiment design:

a write a hypothesis based on your research in Question **4**

b identify the independent, dependent and any controlled variables.

6 The data in the table below was collected for an experiment designed to investigate the effect of temperature on the rate of fermentation in yeast.

Temperature of the water bath (°C)	Time taken to measure the dependent variable (s)
20	328
30	108
40	72
50	155
60	487
70	512

Can you propose an explanation for the observed changes in the dependent variable based on the data collected?

Development of VSEPR theory

The beginnings of VSEPR theory stemmed from the work of Nevil Sidgwick and Herbert Powell who, in 1940, showed that the shape of a molecule was dependent on the total number of electron pairs surrounding a central atom. This concept was refined into a more detailed and useful theory in 1957 by an Australian Professor of Chemistry, Ron Nyholm, and his British colleague, Professor Ronald Gillespie.

CN	number of lone electron pairs							
	0	e.g.	1	e.g.	2	e.g.	3	e.g.
2	linear	CO_2						
3	trigonal planar	BCl_3 SO_3	angled	SO_2 NO_2^- O_3	linear	CO		
4	tetrahedral	CH_4 SO_4^{2-}	trigonal pyramidal	NH_3	angled	H_2O	linear	HCl
5	trigonal bipyramidal	PCl_5	bisphenoidal (seesaw)	SF_4	T-shaped	ClF_3	linear	I_3^-
6	octahedral	SF_6	square pyramidal	ClF_5	square planar	ICl_4^-		
7	pentagonal bipyramidal	IF_7						

FIGURE 16.6.1 VSEPR theory, refined by Nyholm and Gillespie, can be used to predict the shape of molecules.

Prior to the development of VSEPR theory, other models were in use for predicting the shapes of molecules, but as they only took into account the positions of the bonded atoms, they could not accurately predict and explain the shape of every molecule, such as ammonia and water.

VSEPR theory dealt with this problem by accounting for the lone pairs as well as the bonding pairs of electrons, as shown in Figure 16.6.1. While this solved the problem of predicting the shapes of molecules, the theory still could not explain why the bond angles in some molecules deviated from expected bond angles (such as the bond angles in ammonia and water deviating from the tetrahedral bond angles of 109°). Nyholm and Gillespie overcame this by further developing the theory to include rules about the types of electron repulsions and their relative effect; this led to a much better understanding of why and to what extent such bond angle deviations occur.

VSEPR theory's reliance on valence electrons to predict molecular shapes has some limitations. Firstly, it doesn't account for isoelectronic species. Isoelectronic species are elements that have the same number of electrons but exhibit different shapes. Another limitation is that it ignores the relative sizes of substituents in transition metal compounds; this means that it fails to recognise when chemicals are substituted out in a compound. For example, when you replace a hydrogen atom in a hydrocarbon with a chlorine atom, you've introduced a substituent that changes the reactivity and chemical behaviour of the compound, and subsequently the shape. Lastly, VSEPR theory fails to recognise double and triple bonding and therefore treats all bond types equally. Despite these limitations, VSEPR theory remains a useful tool for understanding molecular shape.

KEY QUESTIONS

Forming and finding

1 Discuss why VSEPR theory was an improvement on some of the earlier models for predicting shapes of molecules.

2 Identify the further additions that Nyholm and Gillespie made to the VSEPR theory to make it a better model.

3 Using VSEPR theory, explain the unusual bond angles seen in water.

Analysing

Transition metals (*d* block elements) have high atomic masses and stereochemically inactive lone pairs; this is known as the 'inert pair effect'. The transition metal compounds $[SeCl_6]^{2-}$, $[TeCl_6]^{2-}$ and $[BrF_6]^-$ are predicted to be pentagonal bipyramidal, but they are in fact regular octahedral due to the inert pair effect.

4 What do you think was the dependant variable in this experiment, and how was it measured?

5 What is a possible research question that could explain the process and findings?

Decompression chambers

If you swim at the water's surface, your body experiences a pressure, due to the surrounding air, of about 1 atm. Below the surface, your body experiences an additional pressure due to the water. This additional pressure amounts to about 1 atm for every 10 m of depth. Therefore, at 20 m, the pressure on your body is about 3 atm.

As the pressure on your body increases, the volume of your body cavities such as your lungs and inner ears decreases. This squeezing effect makes diving well below the water's surface without scuba equipment very uncomfortable. Scuba equipment overcomes this problem by supplying air from tanks to the mouth at the same pressure as that produced by the underwater environment.

The pressures felt underwater also affect the way gases behave. As a result of Henry's law, as pressure increases, gases move from the cavities within the body (the lungs) and dissolve into the liquids (the bloodstream). The higher the pressures and colder the water, the faster the dissolving of gases into liquids. As the pressure in a diver's lungs increases during a dive, more gases dissolves in the blood. Nitrogen (N_2) is one of these gases.

When a diver ascends, the pressure drops and the nitrogen becomes less soluble in the blood (according to Henry's law). The nitrogen comes out of solution and can move from the blood back into the cavity (the lungs). Divers are encouraged to breath out as they ascend to further encourage this movement of gases. If a diver ascends too quickly, the rapid pressure drop causes the nitrogen to come out of the blood as tiny bubbles (Figure 16.7.1a). This is like the bubbles of carbon dioxide you observe when you open a bottle of soft drink.

These bubbles cause pain in joints and muscles. If they form in the spinal cord, brain or lungs, they can cause paralysis or death. Treatment for divers suffering from this effect (the bends) involves time in a decompression chamber like the one shown in Figure 16.7.1b.

The chamber increases the pressure surrounding the diver's body, forcing any nitrogen bubbles to dissolve in the blood, and then slowly reduces the pressure back to 1 atm. The duration of treatment depends on the severity of the symptoms, the dive history and the patient's response to treatment.

Hyperbaric oxygen therapy (HBOT) is a medical treatment in which patients breathe pure oxygen while inside a decompression chamber at a pressure higher than 1 atm. Its medical uses include improved wound healing by reduction of swelling, infection control and the stimulation of new blood vessel growth. The hyperbaric unit at the Royal Brisbane and Women's Hospital is equipped with hyperbaric chambers used for treating the bends, ulcers, soft tissue infections, carbon monoxide poisoning and wounds that will not heal, such as those resulting from diabetes or radiotherapy. HBOT is also used by athletes for faster recovery from soft tissue injuries, to produce sharper performance and to maintain more intense training schedules.

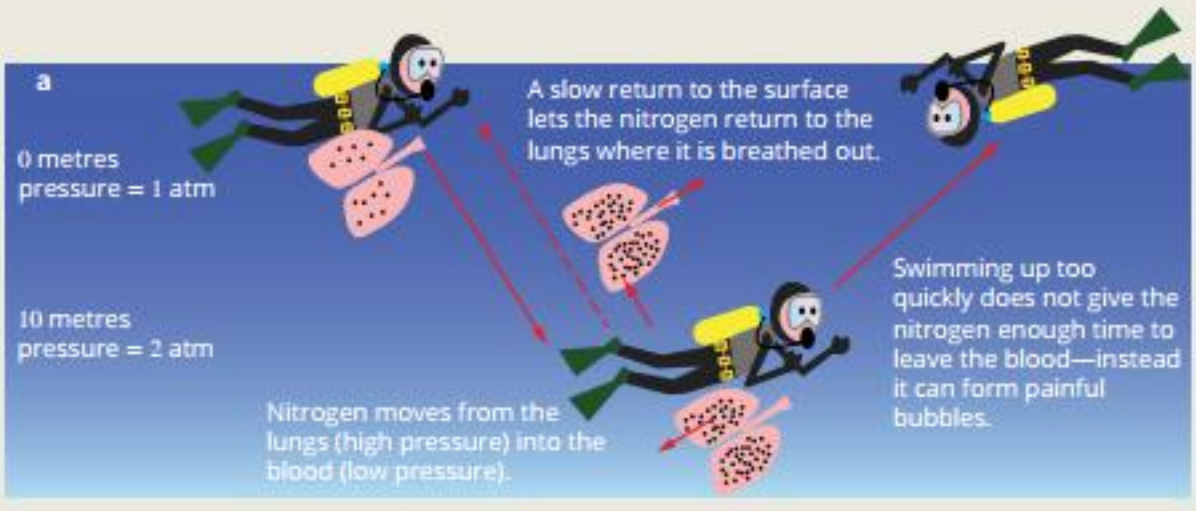

a
0 metres
pressure = 1 atm
10 metres
pressure = 2 atm
A slow return to the surface lets the nitrogen return to the lungs where it is breathed out.
Swimming up too quickly does not give the nitrogen enough time to leave the blood—instead it can form painful bubbles.
Nitrogen moves from the lungs (high pressure) into the blood (low pressure).

FIGURE 16.7.1 (a) Scuba diving and the bends. (b) A decompression chamber is used to treat divers with the bends.

KEY QUESTIONS

Forming and finding

1 Describe HBOT.

2 Explain why it is dangerous for a scuba diver to ascend too quickly and link this to Henry's law.

3 Both temperature and pressure can influence the solubility of gases. Research how the solubility of gases can be affected by temperature, and design an experiment that investigates how temperature can change the rate at which a soft drink goes flat.

Analysing

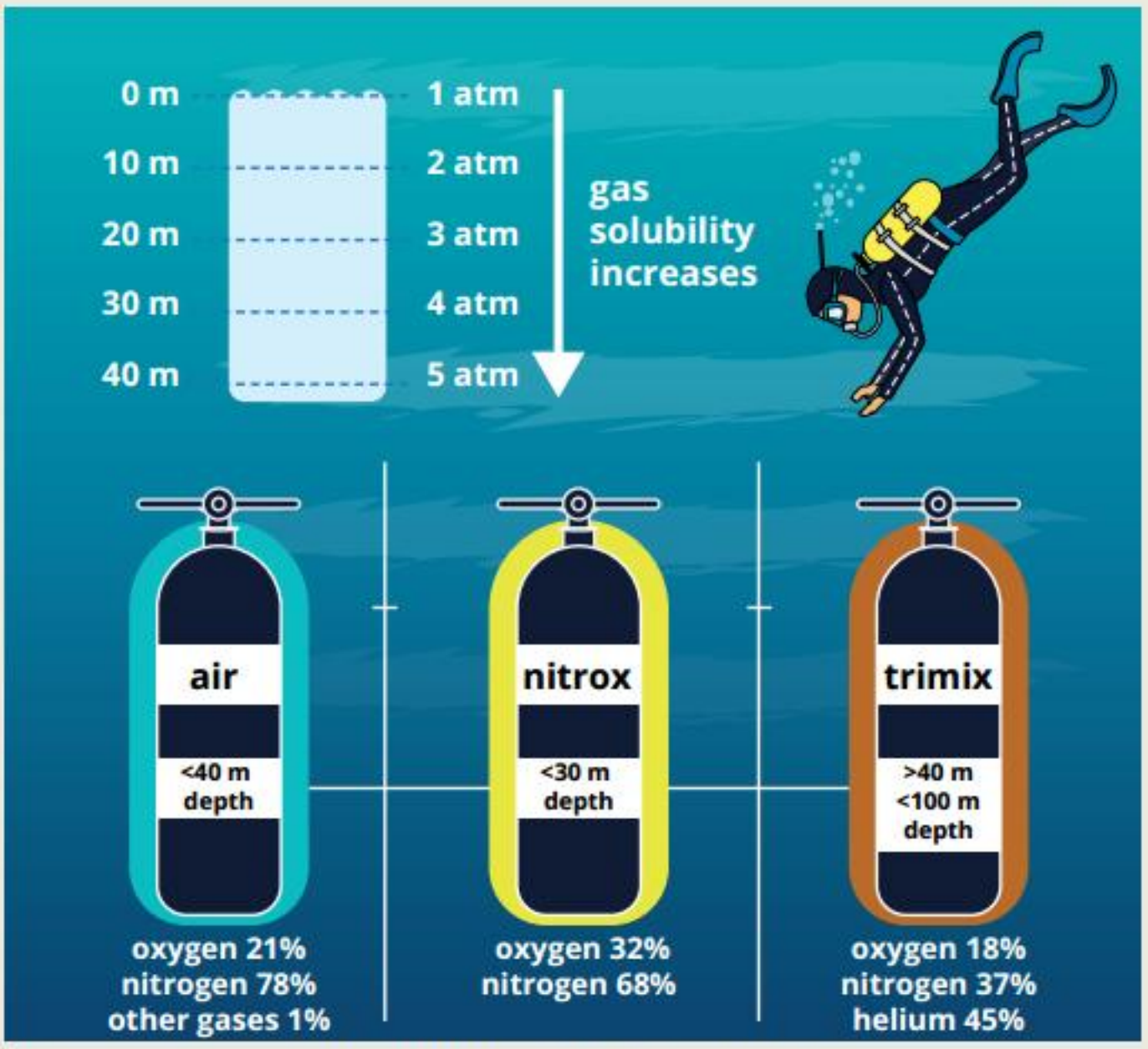


FIGURE 16.7.2 Three types of scuba tanks are predominantly used in diving: air, nitrox and trimix.

Scuba tanks have been designed to combat the behaviour of gases, most notably the negative effects of excess nitrogen in the blood causing the bends. Different gas mixes are used for different depths of dives.

4 How might incorporating data from related studies enhance the validity of the claim that 'gases in scuba tanks are harmful to divers'?

5 Note down any examples of evidence from Figure 16.7.2 that could be included to support the claim.

Blood chemistry

Water's unique properties make it essential to life, particularly its ability to dissolve an enormous range of different solutes. The human body is 66% water by weight. For biological organisms, water provides a system to transport nutrients and soluble wastes. It also transports essential reactants for chemical reactions to cells and tissues.

The circulatory system of the body forms a transportation network (Figure 16.8.1). Blood plasma is an aqueous solution containing a range of ionic and molecular substances, which enables essential nutrients, ions and molecules dissolved in water to be carried to your organs, brain and tissues. The flow of blood through the circulatory system also carries away waste products.

FIGURE 16.8.1 The circulatory system of the body transports many ions and molecules dissolved in water. The solute particles include nutrients and waste products from the body's metabolic processes.

Blood is a suspension of red blood cells, white blood cells and plasma (Figure 16.8.2). Plasma makes up over 90% of the blood and contains mostly water. This water acts as a solvent for carrying other substances throughout the circulatory system.

FIGURE 16.8.2 Centrifuging blood separates it into clear layers, demonstrating that blood is actually a heterogeneous suspension. Here you can see the plasma on top and the red blood cells on the bottom.

Glucose is a monosaccharide used to produce energy in all cells via cellular respiration. It is therefore essential that glucose can be transported around the body in the bloodstream. Glucose has many hydroxyl functional groups that form hydrogen bonds with water (Figure 16.8.3).

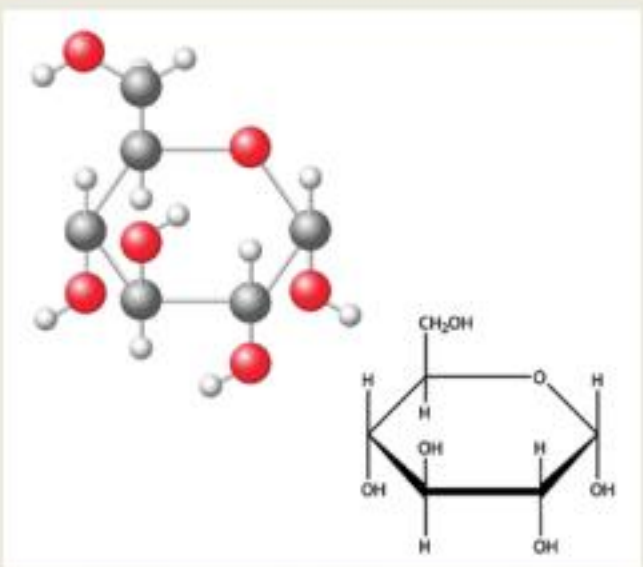


FIGURE 16.8.3 The molecular structure of glucose (the sugar found in our blood). It can dissolve in water because of the presence of polar –OH groups.

Proteins are polar molecules made up of amino acids. Amino acids have polar regions, some of which can form hydrogen bonds with water, while other regions can form dipole–dipole interactions. These interactions allow proteins to dissolve readily in the water in plasma. These proteins may be hormones like insulin, which is produced in the pancreas. Insulin triggers cells to uptake more glucose from the bloodstream to maintain blood sugar levels.

Sodium and potassium are important minerals necessary for the transmission of nerve impulses and also need to be transported around the body. The ions dissolve readily by forming **ion–dipole interactions** with the water molecules in plasma.

Vitamins are organic compounds that are required in the diet for the body to function properly and help to prevent specific diseases. For example, a deficiency of vitamin K can lead to uncontrolled bleeding and a deficiency of vitamin C can lead to scurvy. Someone with scurvy suffers from fatigue, swollen and bleeding gums and open sores. Unlike proteins and carbohydrates, vitamins do not share a common structure. Instead, vitamins are classified as fat soluble or water soluble. The differences in solubility relate to the number and type of functional groups in the molecule, such as the hydroxyl group, which can form hydrogen bonds with water. The more of these groups there are in a vitamin molecule, the higher its solubility in water. Fat-soluble vitamins have proportionally fewer functional groups, making the molecules relatively non-polar. These non-polar vitamins can form dispersion forces with the lipids in the fat tissue of the body.

The solubility of vitamins has implications for humans. Water-soluble vitamins are excreted by the body if not used, so they must be consumed as a regular part of the diet. By contrast, fat-soluble vitamins can be stored in the body, in fatty tissue, for long periods of time. If the diet is deficient in a particular fat-soluble vitamin, the stored reserves are available for use.

KEY QUESTIONS

Forming and finding

1 Identify the key interactions that allow water to act as a solvent for carrying other substances throughout the circulatory system.

2 Antibodies are important biological proteins that fight infections against invading pathogens such as varicella (which causes chicken pox) in the human body. Calcium is an important mineral needed for muscle contraction. Distinguish between the ways in which these substances dissolve in blood plasma.

3 If a person consumes too much vitamin supplement, over time they can develop a potentially dangerous condition called hypervitaminosis. Find one scientifically credible source, such as a podcast from the last six months or an article from a popular science website, to describe this condition and suggest why this condition is more likely to occur for vitamin A than vitamin C. List the reference using appropriate referencing citations.

Analysing

4 Some hormones, such as oestrogen and testosterone, are composed of lipids, which are non-polar biomacromolecules. Discuss how these hormones interact with the watery component of blood plasma and how they travel around the body.

5 Vitamin C and the B vitamins (e.g. vitamin B12) are water-soluble vitamins. What implications does this have for food preparation?

Acid rain

Sulfur dioxide (SO_2) is a gas produced during the combustion of fossil fuels containing sulfur impurities. Most sulfur dioxide released into the atmosphere comes from burning coal or oil in electric power stations. When these fuels burn, the chemical reaction yields SO_2, which then dissolves in water to form an acidic solution.

$$S(s) + O_2(g) \rightarrow SO_2(g)$$

The sulfur dioxide is converted to sulfuric acid via a series of reactions that occur in the atmosphere:

$$SO_2(g) \rightarrow SO_3(g) \rightarrow H_2SO_4 \text{ (in rain)}$$

The dissociation reactions of H_2SO_4 and HSO_4^- with water produce the hydronium ion, which is the defining characteristic of acids. These dissociation reactions are represented by the following equations:

$$H_2SO_4(l) + H_2O(l) \rightarrow HSO_4^-(aq) + H_3O^+(aq)$$

$$HSO_4^-(aq) + H_2O(l) \rightleftharpoons SO_4^{2-}(aq) + H_3O^+(aq)$$

The sulfuric acid in acid rain reacts with metal carbonates to produce a salt, carbon dioxide and water—a reaction discussed in Module 14.3—and its effects are commonly seen in limestone buildings rich in calcium carbonate (Figure 16.9.1). Acid rain can also cause metal structures to degrade more quickly, increasing the rate of oxidation of metals to metal salts—which is another reaction discussed in Module 14.3.

FIGURE 16.9.1 This limestone wall has been corroded by acid rain, causing the cavities.

Since the early 1990s, most countries have taken steps to reduce acid rain, with stricter government regulations and international treaties aimed at reducing the emissions of sulfur dioxide and nitrogen oxides. These regulations have had great successes in decreasing the concentration of these gases over recent years. Industries were encouraged to significantly reduce emissions through the use of alternative fuels and the inclusion of sulfur scrubbers, also known as flue gas desulfurization (FGD) systems.

Sulfur dioxide can be removed from waste gases in factories by treating the gases with limestone to form calcium sulfate. This can then be used to make plasterboard, which lines the internal walls of buildings.

The CSIRO states that because of Australia's sparse population and widely spread emission sources, Australia's acid rain levels are relatively low. Australian coal is also very low in sulfur, further contributing to lower levels of acid rain seen in this country. Countries such as Russia, India and China are limited in both space and the availability of low-sulfur coal. Instead, there is still a heavy reliance on high-sulfur coal.

KEY QUESTIONS

Forming and finding

1 Explain how the sulfur content of burning coal can affect the formation of acid rain.

2 Summarise the forming of acid rain.

3 What possible methods from the text in the article could be used to help reduce SO_2 levels in Russia, China and India?

4 Find one scientifically credible source, such as a podcast from the last six months or an article from a popular science website, that extends your knowledge on this topic, and state what makes it a credible source.

Analysing

Scientists in China set about recording the pH of the average rainfall for the country and matched it to the sulfur dioxide emissions from the country's many coal-fired power stations. The results are shown in the Figure 16.9.2.

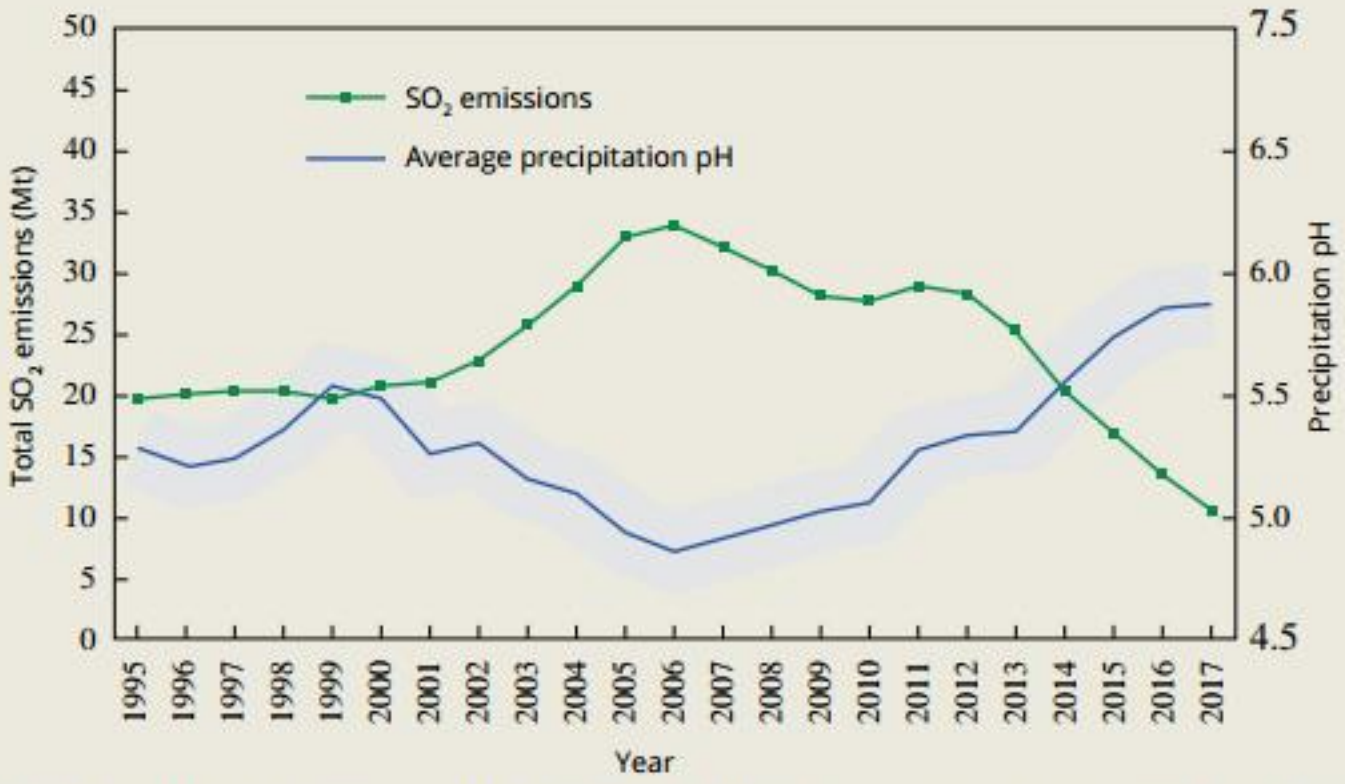


FIGURE 16.9.2 Trends in the Chinese national average precipitation pH and total SO_2 emissions between 1995 and 2017 (Lu, *et al.*, 2020)

5 Can you identify specific patterns or trends in the data related to the dependent variable?

6 Propose an explanation for the observed changes seen after 2010 in the dependent variable based on the data analysis?

Water quality

In 2016, the city of Flint in Michigan, USA, switched its water source from Lake Huron to the relatively unmonitored Flint River to save on costs. The river water was more corrosive due to its higher chloride content and lower pH compared to the previous source from the lake. When water with low pH (acidic) or high salinity comes into contact with lead-containing pipes, it can cause the pipes to corrode. Normally, water treatment facilities add corrosion inhibitors (such as orthophosphate) to prevent this leaching; however, this was not done.

FIGURE 16.10.1 Water collected from residents' homes in Flint, Michigan, as part of the research done by FlintWaterStudy.org on the Flint water crisis (Reilly, 2016)

The corrosion process involves the dissolution of lead ions (Pb^{2+}) from the pipes into the water and subsequently into people's homes.

$$Pb(s) \rightarrow Pb^{2+}(aq) + 2e^-$$

Many cases of lead poisoning, rashes, hair loss and an outbreak of Legionnaires' disease triggered a public outcry that something was wrong with the water supply. At first, the government refused to acknowledge the event, and so it fell on independent scientists, teachers and students to gather data from water samples to prove that leaching was occurring (Figure 16.10.1).

Gravimetric analysis is a technique that can be used to determine the amount dissolved lead (Pb^{2+}) present in a solution. Potassium iodide (KI) reacts with lead ions in a double displacement precipitation reaction to form the insoluble salt lead(II) iodide (PbI_2)

$2KI(aq) + Pb(NO3)_2(aq) \rightarrow 2KNO_3(aq) + PbI_2(s)$

Using the stoichiometric ratios in the above equation, and measuring the mass of precipitate formed, allows calculation of the concentration of dissolved lead (Pb^{2+}).

In Flint, scientists used an Inductively Coupled Plasma Mass Spectrometer (ICP-MS), a machine that can measure elements at trace levels in sampled solutions, to measure the amount of lead in samples of tap water collected from residents' homes. The levels of lead were found to be significantly higher than the allowed limit.

In response to these findings, the city of Flint installed six water quality monitoring stations across different areas that provided real-time water quality assessments of the river.

Salts are ionic compounds and dissociate in water, forming ion–dipole interactions with the water molecules. Pure water is a poor conductor of electricity as there are no charged particles available to carry a current. The conductivity of water increases with more ions dissolved in the water. Measuring the conductivity of a water sample gives an indication of the number of dissolved salts in the water.

In Australia, water authorities are required to provide water suitable for drinking purposes. This requires regular monitoring of water quality from catchment areas and throughout the various stages of treatment, storage and delivery. The concentration of common ions like sodium, calcium and potassium, as well as nutrients like phosphate and nitrogen, are routinely tested.

KEY QUESTIONS

Forming and finding

1 Distinguish between gravimetric analysis and Inductively Coupled Plasma Mass Spectrometry (ICP-MS).

2 Explain how collecting water samples from several locations along the Flint River might affect water quality results and the way that the water is treated or used.

3 Find one scientifically credible source, such as a podcast from the last six months or an article from a popular science website, that extends your knowledge about the Flint water crisis. List the reference, using appropriate referencing citations, and evaluate the reliability of the source you have found.

Analysing

Data from independent testing of water samples collected from the homes of Flint were compiled from several companies and independent citizen scientists, with a focus on water lead levels (WLL). The data was compared to the national minimum reporting level (MRL) and the action level (AL) as set by the USEPA. The data are shown in Table 16.10.1. First draw refers to a sample taken as soon as the tap is turned on. A 1-minute draw is a sample taken after the tap has been running for 1 minute.

TABLE 16.10.1 Water lead levels for each sample campaign between August 2015 and August 2017 (Pieper et al., 2018)

		Number of samples	Median WLL ($\mu g L^{-1}$)	90th percentile WLL ($\mu g L^{-1}$)	Per cent above AL[a]	Max WLL ($\mu g L^{-1}$)
August 2015	First draw	268	3.5	26.8	17%	158.0
	1-minute draw		1.4	11.3	6%	1051.0
	3-minute draw		<MRL	6.6	4%	94.5
March 2016	First draw	186	1.9	24.5	16%	2253.0
	1-minute draw		<MRL	9.0	5%	286.3
	3-minute draw		<MRL	3.4	2%	69.0
July 2016	First draw	176	1.2	15.1	10%	337.3
	1-minute draw		<MRL	5.7	3%	94.0
	3-minute draw		<MRL	3.3	3%	67.5
November 2016	First draw	164	<MRL	9.2	7%	82.3
	1-minute draw		<MRL	3.9	2%	219.2
	3-minute draw		<MRL	2.8	1%	1740.0
August 2017	First draw	150	<MRL	9.0	7%	221.2
	1-minute draw		<MRL	3.0	3%	51.8
	3-minute draw		<MRL	2.2	<1%	132.9

[a]AL: USEPA action level of $15 \mu g L^{-1}$

Minimum reporting level (MRL) for lead = $1 \mu g L^{-1}$

WLL: water lead level

4 Can you identify specific patterns or trends in the data related to the dependent variable?

5 Identify a possible limitation that might result from the gathering of this data.

APPENDIX A Symbols, units and fundamental constants

TABLE 1 Units and symbols based on the SI system*

Quantity	Symbol for physical quantity	Corresponding SI unit	Symbol for SI unit	Definition of SI unit
Mechanics				
length	*l*	metre	m	fundamental unit
area	*A*	square metre	m^2	
volume	*V*	cubic metre	m^3	
mass	*m*	kilogram	kg	fundamental unit
density	*d*	–	$kg\,m^{-3}$	
time	*T*	second	s	fundamental unit
force	*F*	newton	N	$kg\,m\,s^{-2}$
pressure	*P*	pascal	Pa	$N\,m^{-2}$
energy	*E*	joule	J	N m
Electricity				
electric current	*I*	ampere	A	fundamental unit
electric charge	*Q*	coulomb	C	A s
electric potential difference	*V*	volt	V	$J\,A^{-1}\,s^{-1}$
Nuclear and chemical quantities				
atomic number	*Z*	–	–	–
mass number	*A*	–	–	–
amount of substance	*n*	mole	mol	fundamental unit
particle number	*N*	–	–	–
relative atomic mass	A_r	–	–	–
relative molecular mass	M_r	–	–	–
molar mass	*M*	–	–	$kg\,mol^{-1}$
molar volume	V_m	–	–	$m^3\,mol^{-1}$
concentration	*c*	–	–	$mol\,dm^{-3}$ or $mol\,L^{-1}$
Thermal quantities				
Temperature	*T*	kelvin	K	fundamental unit
specific heat capacity	*c*	–	–	$J\,kg^{-1}\,K^{-1}$

*Units listed in red are the arbitrarily defined fundamental units of the SI system.

TABLE 2 SI prefixes, their symbols and values

SI prefix	Symbol	Value
pico	p	10^{-12}
nano	n	10^{-9}
micro	μ	10^{-6}
milli	m	10^{-3}
centi	c	10^{-2}
deci	d	10^{-1}
kilo	k	10^{3}
mega	M	10^{6}
giga	G	10^{9}
tera	T	10^{12}

TABLE 3 Physical constants and values

Description	Symbol	Value
Avogadro's constant	N_A	$6.02 \times 10^{23}\,mol^{-1}$
mass of electron	m_e	$9.109 \times 10^{-31}\,kg$
mass of proton	m_p	$1.673 \times 10^{-27}\,kg$
mass of neutron	m_n	$1.675 \times 10^{-27}\,kg$
gas constant	*R*	$8.31\,J\,mol^{-1}\,K^{-1}$
ionic product for water	K_w	$1.0 \times 10^{-14}\,mol^2\,L^{-2}$ at 298 K
molar volume of an ideal gas (at STP)	V_m	$2.27 \times 10^{-2}\,m^3\,mol^{-1}$; $22.7\,dm^3\,mol^{-1}$; $22.7\,L\,mol^{-1}$
specific heat capacity of water	*C*	$4.18\,J\,g^{-1}\,K^{-1}$
density of water	*d*	$1.00\,g\,mL^{-1}$ at 298 K
temperature in kelvin	T_k	T°C + 273
standard temperature and pressure	STP	273 K and 100 kPa

APPENDIX B Table of relative atomic masses

TABLE 1 Table of relative atomic masses*

Element name	Symbol	Atomic number	Relative atomic mass
actinium	Ac	89	–
aluminium	Al	13	26.98
americium	Am	95	–
antimony	Sb	51	121.76
argon	Ar	18	39.95
arsenic	As	33	74.92
astatine	At	85	–
barium	Ba	56	137.33
berkelium	Bk	97	–
beryllium	Be	4	9.01
bismuth	Bi	83	208.98
bohrium	Bh	107	–
boron	B	5	10.81
bromine	Br	35	79.90
cadmium	Cd	48	112.41
caesium	Cs	55	132.91
calcium	Ca	20	40.08
californium	Cf	98	–
carbon	C	6	12.01
cerium	Ce	58	140.12
chlorine	Cl	17	35.45
chromium	Cr	24	52.00
cobalt	Co	27	58.93
copernicium	Cn	112	–
copper	Cu	29	63.55
curium	Cm	96	–
darmstadtium	Ds	110	–
dubnium	Db	105	–
dysprosium	Dy	66	162.50
einsteinium	Es	99	–
erbium	Er	68	167.26
europium	Eu	63	151.96
fermium	Fm	100	–
flerovium	Fl	114	–
fluorine	F	9	19.00
francium	Fr	87	–
gadolinium	Gd	64	157.25
gallium	Ga	31	69.72
germanium	Ge	32	72.63
gold	Au	79	196.97
hafnium	Hf	72	178.49
hassium	Hs	108	–
helium	He	2	4.00
holmium	Ho	67	164.93
hydrogen	H	1	1.01
indium	In	49	114.82
iodine	I	53	126.90
iridium	Ir	77	192.22
iron	Fe	26	55.85
krypton	Kr	36	83.80
lanthanum	La	57	138.91
lawrencium	Lr	103	–
lead	Pb	82	207.22
lithium	Li	3	6.94
livermorium	Lv	116	–
lutetium	Lu	71	174.97
magnesium	Mg	12	24.31
manganese	Mn	25	54.94
meitnerium	Mt	109	–
mendelevium	Md	101	–
mercury	Hg	80	200.59
molybdenum	Mo	42	95.95
moscovium	Mc	115	–
neodymium	Nd	60	144.24
neon	Ne	10	20.18
neptunium	Np	93	–
nickel	Ni	28	58.69
nihonium	Nh	113	–
niobium	Nb	41	92.91
nitrogen	N	7	14.01
nobelium	No	102	–
oganesson	Og	118	–
osmium	Os	76	190.2
oxygen	O	8	16.00
palladium	Pd	46	106.42
phosphorus	P	15	30.97
platinum	Pt	78	195.08
plutonium	Pu	94	–
polonium	Po	84	–
potassium	K	19	39.10
praseodymium	Pr	59	140.98
promethium	Pm	61	–
protactinium	Pa	91	231
radium	Ra	88	–
radon	Rn	86	–
rhenium	Re	75	186.21
rhodium	Rh	45	102.91
roentgenium	Rg	111	–
rubidium	Rb	37	85.47
ruthenium	Ru	44	101.07
rutherfordium	Rf	104	–
samarium	Sm	62	150.4
scandium	Sc	21	44.96
seaborgium	Sg	106	–
selenium	Se	34	78.97
silicon	Si	14	28.09
silver	Ag	47	107.87
sodium	Na	11	22.99
strontium	Sr	38	87.62
sulfur	S	16	32.06
tantalum	Ta	73	180.95
technetium	Tc	43	–
tellurium	Te	52	127.60
tennessine	Ts	117	–
terbium	Tb	65	158.93
thallium	Tl	81	204.38
thorium	Th	90	232.04
thulium	Tm	69	168.93
tin	Sn	50	118.71
titanium	Ti	22	47.87
tungsten	W	74	183.84
uranium	U	92	238.03
vanadium	V	23	50.942
xenon	Xe	54	131.29
ytterbium	Yb	70	173.05
yttrium	Y	39	88.91
zinc	Zn	30	65.38
zirconium	Zr	40	91.22

*Based on the atomic mass of $^{12}C = 12$.
The values for relative atomic masses given in the table apply to elements as they exist in nature (without artificial alteration of their isotopic composition) and to natural mixtures that do not include isotopes of radiogenic origin.

APPENDIX C Electronegativities and first ionisation energy of selected elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 **H** 2.2 1318																	2 **He** 2379
3 **Li** 1.0 526	4 **Be** 1.6 906											5 **B** 2.0 807	6 **C** 2.6 1093	7 **N** 3.0 1407	8 **O** 3.4 1320	9 **F** 4.0 1687	10 **Ne** 2087
11 **Na** 0.9 502	12 **Mg** 1.3 744											13 **Al** 1.6 584	14 **Si** 1.9 793	15 **P** 2.2 1018	16 **S** 2.6 1006	17 **Cl** 3.2 1257	18 **Ar** 1527
19 **K** 0.8 425	20 **Ca** 1.0 596	21 **Sc** 1.4 637	22 **Ti** 1.5 664	23 **V** 1.6 656	24 **Cr** 1.7 659	25 **Mn** 1.6 724	26 **Fe** 1.8 766	27 **Co** 1.9 765	28 **Ni** 1.9 743	29 **Cu** 1.9 752	30 **Zn** 1.7 913	31 **Ga** 1.8 585	32 **Ge** 2.0 768	33 **As** 2.2 953	34 **Se** 2.6 947	35 **Br** 3.0 1146	36 **Kr** 2.9 1357
37 **Rb** 0.8 409	38 **Sr** 1.0 556	39 **Y** 1.2 606	40 **Zr** 1.3 666	41 **Nb** 1.6 670	42 **Mo** 2.2 691	43 **Tc** 1.9 708	44 **Ru** 2.2 717	45 **Rh** 2.3 726	46 **Pd** 2.2 811	47 **Ag** 1.9 737	48 **Cd** 1.7 874	49 **In** 1.8 565	50 **Sn** 2.0 715	51 **Sb** 2.0 840	52 **Te** 2.1 876	53 **I** 2.7 1015	54 **Xe** 2.6 1177
55 **Cs** 0.8 382	56 **Ba** 0.9 509																

Atomic Number

Symbol
electronegativity
first ionisation energy (kJ mol^{-1})

Groups in accordance with IUPAC numbering.

Atomic radius ($\times 10^{-12}$m)
Symbol
Ionic radius (charge of ion)

32 **H** 208 (1–)																	37 **He**
130 **Li** 76 (1+)	99 **Be** 45 (2+)											84 **B** 27 (3+)	75 **C** 16 (4+)	71 **N** 146 (3–)	64 **O** 140 (2–)	60 **F** 133 (1–)	62 **Ne**
160 **Na** 102 (1+)	140 **Mg** 72 (2+)											124 **Al** 53 (3+)	114 **Si** 40 (4+)	109 **P** 38 (5+)	104 **S** 184 (2–)	100 **Cl** 181 (1–)	101 **Ar**
200 **K** 138 (1+)	174 **Ca** 100 (2+)	159 **Sc** 75 (3+)	148 **Ti** 86 (2+) 61 (4+)	144 **V** 79 (2+) 54 (5+)	130 **Cr** 62 (3+) 44 (6+)	129 **Mn** 83 (2+) 64 (3+)	124 **Fe** 78 (2+) 64 (3+)	118 **Co** 74 (2+) 61 (3+)	117 **Ni** 69 (2+) 60 (3+)	122 **Cu** 77 (1+) 73 (2+)	120 **Zn** 74 (2+)	123 **Ga** 62 (3+)	120 **Ge** 53 (4+) 272 (4–)	120 **As** 58 (3+) 46 (5+)	118 **Se** 198 (2–)	117 **Br** 196 (1–)	116 **Kr**
215 **Rb** 152 (1+)	190 **Sr** 118 (2+)	176 **Y** 90 (3+)	164 **Zr** 72 (4+)	156 **Nb** 64 (5+)	148 **Mo** 65 (4+)	138 **Tc** 65 (4+)	136 **Ru** 62 (4+)	134 **Rh** 67 (3+)	130 **Pd** 86 (2+)	136 **Ag** 115 (1+)	140 **Cd** 95 (2+)	142 **In** 80 (3+)	140 **Sn** 69 (4+)	140 **Sb** 76 (3+)	137 **Te** 221 (2–)	136 **I** 220 (1–)	136 **Xe**
238 **Cs** 167 (1+)	206 **Ba** 135 (2+)																

APPENDIX E Indicators and their pH range and pK_a value

Indicator	pH range	pK_a
methyl violet	0.0–1.6	–
thymol blue	1.2–2.8	1.7
methyl orange	3.1–4.4	3.7
bromophenol blue	3.0–4.6	3.8
bromocresol green	3.8–5.4	4.7
methyl red	4.4–6.2	5.1
bromothymol blue	6.0–7.6	7.0
phenol red	6.8–8.4	7.9
phenolphthalein	8.3–10.0	9.6
alizarin yellow	10.1–12.0	11.2

APPENDIX F Formulas and charges for common ions

Positive ions (cations)						Negative ions (anions)			
1+		2+		3+		1–		2–	
caesium	Cs^+	barium	Ba^{2+}	aluminium	Al^{3+}	acetate (ethanoate)	CH_3COO^-	carbonate	CO_3^{2-}
copper(I)	Cu^+	cadmium(II)	Cd^{2+}	chromium(III)	Cr^{3+}	bromide	Br^-	chromate	CrO_4^{2-}
gold(I)	Au^+	calcium	Ca^{2+}	gold(III)	Au^{3+}	chloride	Cl^-	dichromate	$Cr_2O_7^{2-}$
lithium	Li^+	cobalt(II)	Co^{2+}	iron(III)	Fe^{3+}	cyanide	CN^-	hydrogen phosphate	HPO_4^{2-}
potassium	K^+	copper(II)	Cu^{2+}			dihydrogen phosphate	$H_2PO_4^-$	oxalate	$C_2O_4^{2-}$
rubidium	Rb^+	iron(II)	Fe^{2+}	4+		fluoride	F^-	oxide	O^{2-}
silver	Ag^+	lead(II)	Pb^{2+}	lead(IV)	Pb^{4+}	hydrogen carbonate	HCO_3^-	peroxide	O_2^{2-}
sodium	Na^+	magnesium	Mg^{2+}	tin(IV)	Sn^{4+}	hydrogen sulfate	HSO_4^-	sulfate	SO_4^{2-}
ammonium	NH_4^+	manganese(II)	Mn^{2+}			hydrogen sulfide	HS^-	sulfide	S^{2-}
hydronium	H_3O^+	mercury(II)	Hg^{2+}			hydrogen sulfite	HSO_3^-	sulfite	SO_3^{2-}
		nickel	Ni^{2+}			hydroxide	OH^-	thiosulfate	$S_2O_3^{2-}$
		strontium	Sr^{2+}			hypochlorite	ClO^-	3–	
		tin(II)	Sn^{2+}			iodide	I^-	citrate	$C_6H_5O_7^{3-}$
		zinc	Zn^{2+}			nitrate	NO_3^-	nitride	N^{3-}
						nitrite	NO_2^-	phosphate	PO_4^{3-}
						perchlorate	ClO_4^-	phosphide	P^{3-}
						permanganate	MnO_4^-		

APPENDIX G Solubilities of ionic compounds at 298 K

	bromide	carbonate	chloride	hydroxide	iodide	nitrate	oxide	phosphate	sulfate
aluminium	s	–	s	i	s	s	i	i	s
ammonium	s	s	s	s	s	s	–	s	s
barium	s	i	s	s	s	s	s	i	i
calcium	s	i	s	p	s	s	p	i	p
cobalt(II)	s	i	s	i	s	s	i	i	s
copper(II)	s	–	s	i	i	s	i	i	s
iron(II)	s	i	s	i	s	s	i	i	s
iron(III)	s	–	s	i	s	s	i	i	s
lead(II)	p	i	s	i	i	s	i	i	i
lithium	s	s	s	s	s	s	s	–	s
magnesium	s	i	s	i	s	s	i	p	s
manganese(II)	s	i	s	i	s	s	i	p	s
potassium	s	s	s	s	s	s	s	s	s
silver	i	i	i	i	i	s	i	i	p
sodium	s	s	s	s	s	s	s	s	s
zinc	s	i	s	i	s	s	i	i	s

s = soluble in water (solubility greater than 10 g L^{-1})
p = partially soluble in water (solubility between 1 and 10 g L^{-1})
i = insoluble in water (solubility less than 1 g L^{-1})
– = no data

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Appendices are reflective of the 2025 QCAA syllabus.

APPENDIX H Average bond enthalpies at 298 K

TABLE 1 Average bond enthalpies ($kJ\,mol^{-1}$) for single bonds at 25°C and 1 atm pressure

	H	C	N	O	F	S	Cl	Br	I
H	436								
C	414	346							
N	391	286	158						
O	463	358	214	144					
F	567	492	278	191	159				
S	364	289			327	266			
Cl	431	324	192	206	255	271	242		
Br	366	285		201	249	218	219	193	
I	298	228		201	280		211	178	151

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TABLE 2 Average bond enthalpies ($kJ\,mol^{-1}$) for multiple bonds at 25°C and 1 atm pressure

C=C	614
C≡C	839
C=N	615
C≡N	890
C=O	804
N=N	470
N≡N	945
O=O	498

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Glossary

A

absolute uncertainty The uncertainty of a measurement expressed in the same units as the measurement.

absorption spectrum A spectrum produced when an element absorbs radiation, and electrons move from a lower energy level to a higher energy level. It appears as distinct lines characteristic of the element.

accuracy The quality of being true, correct or precise, representing the extent to which a measurement reflects the actual quantity being measured. In science, accuracy requires both obtaining a measurement close to the true value and providing an estimate of uncertainty. Achieving accurate results requires minimising systematic errors to ensure the measurement reliably captures the intended quantity.

acid (Arrhenius acid) A substance that, when dissolved in water, ionises to produce the hydrogen ion, H^+, thereby increasing the H^+ ion concentration of the solution.

acid (Brønsted–Lowry acid) A substance that donates a hydrogen ion (proton) to another substance in a proton transfer reaction.

acid rain Rainwater that has reacted with acidic emissions from industry and vehicles and has a pH less than 5.5.

acid–base reaction A reaction in which one substance, an acid, donates a hydrogen ion (proton) to another substance, a base.

acidic solution An aqueous solution in which the concentration of hydronium ions (H_3O^+) is greater than the concentration of hydroxide ions (OH^-). At 25°C, pH < 7.

acidity The concentration of H_3O^+ ions in an aqueous solution. Acidity is measured using the pH scale.

activation energy The minimum energy required by reactants for a reaction to occur; E_a. This energy is needed to break the bonds between atoms in the reactants to allow products to form.

actual yield The mass of product actually obtained during a chemical reaction. This will be less than or equal to the theoretical yield.

adsorption The attraction and binding of molecules or particles of one substance to the surface of another.

alkali A soluble base or a solution of a soluble base.

alkali metal A group 1 metal—Li, Na, K, Rb, Cs and Fr.

alkaline earth metals A group 2 metal—Be, Mg, Ca, Sr, Ba and Ra.

allotrope Different forms of the same element in which the atoms combine in different ways.

alloy A substance formed when other materials (e.g. carbon, other metals) are mixed with a metal.

alpha particle A particle composed of two protons and two neutrons, also known as a helium nucleus.

amino acids The monomer molecule used to make proteins.

amphiprotic A substance that has the ability to act as an acid (donate a proton or hydrogen ions) and also to act as a base (accept a proton and hydrogen ions). All amphiprotic substances are amphoteric. Not all amphoteric substances are amphiprotic.

amphoteric The ability to act as an acid and also as a base.

anion A negatively charged ion, e.g. a chloride ion, Cl^-.

anomaly Deviation from what is expected or considered to be normal or standard.

aqueous When a chemical species has been dissolved in water, the resulting solution is said to be aqueous. This can be shown by writing '(aq)' after the name or symbol of the chemical.

aqueous solution A solution in which water is the solvent. Typically represented with the (aq) after the chemical formula of the solute, e.g. NaCl(aq) represents the solute sodium chloride dissolved in water.

asymmetrical molecule A molecule in which the polar bonds are unevenly (or asymmetrically) distributed. The bond dipoles do not cancel out and a net dipole is formed.

atom The basic building block of matter. It is made up of subatomic particles—protons, neutrons and electrons.

atomic absorption spectroscopy (AAS) An analytical technique that uses light absorption to identify a metal in a sample and produces qualitative results.

atomic absorption spectrometry (AAS) An analytical technique that uses light absorption to measure the concentration of a metal in a sample and produces quantitative results.

atomic mass The mass of an atom in atomic mass units (amu).

atomic mass unit (amu) One atomic mass unit is defined as a mass exactly equal to $\frac{1}{12}$ the mass of a ^{12}C atom.

atomic number The number of protons in an element's nucleus, Z; in a neutral atom, the number of protons will be equal to the number of electrons orbiting the nucleus.

atomic radius A measurement used for the size of atoms; the distance from the nucleus to the outermost electrons.

atomic theory of matter The proposal made by John Dalton that all matter is composed of atoms.

Aufbau principle The explanation of the most stable electron arrangement in an atom; electrons fill lower energy shells and subshells before residing in higher energy shells and subshells.

average bond enthalpy The average energy, taken across a wide variety of different molecules, required to break a specific type of bond.

average rate of reaction The change in concentration of a reactant or product per unit time measured between two different time points during a chemical reaction.

Avogadro's constant The number of particles in a mole; symbol $N_A = 6.02 \times 10^{23}$ mol^{-1}.

Avogadro's number The fixed numerical value of Avogadro's constant: 6.02×10^{23}. The number of particles in a mole.

B

balanced equation The number of each type of atom on the reactant side of the equation equals the number of each type of atom on the product side.

Balmer series A series of spectral lines in the visible part of the hydrogen spectrum that is produced by transitions of electrons between the n = 2 energy level and higher energy levels of the hydrogen atom.

bar graph A graph that shows the measured value of the dependent variable by the length of a horizontal bar.

base (Arrhenius base) A substance that, when dissolved in water, dissociates to produce the hydroxide ion, OH^-, thereby increasing the OH^- ion concentration of the solution.

base (Brønsted–Lowry base) A substance that accepts a hydrogen ion (proton) from another substance in a proton transfer reaction.

basic solution An aqueous solution in which the concentration of hydronium ions (H_3O^+) is less than the concentration of hydroxide ions (OH^-). For a basic solution at 25°C, pH > 7.

beta radiation Electrons emitted by radioactive decay.

bias An inclination or prejudice towards something. In measurement, when measured values are consistently higher or consistently lower than the true value.

binary molecular compound A compound comprised of atoms from only two types of non-metallic elements.

block (periodic table) One of four main parts of the periodic table where elements have the same highest energy subshell filled, i.e. *s*, *p*, *d* or *f* subshell.

Bohr diagram A diagram that shows the arrangement of electrons in shells around the nucleus.

Bohr model The description of each electron in an atom as occupying a discrete energy level in the region around the nucleus; the movement of electrons to a different energy level involves absorbing or emitting energy. The Bohr model is also referred to as the shell model.

boiling point The temperature at which the vapour pressure of a liquid equals the external pressure on the surface of liquid. The boiling point is therefore dependent on the external pressure. It is typically characterised by the escape of gaseous bubbles of a substance from the liquid state of the substance.

boiling point elevation The increase in temperature between the boiling point of a solution and the boiling point of the pure solvent.

bond angle The angle formed between adjacent bonds on a central atom.

bond enthalpy The energy needed to break one mole of bonds of gaseous molecules under standard conditions.

bonding electrons The electrons used to form a covalent bond.

bonding pairs A pair of electrons that is shared between two atoms to form a covalent bond.

brittle Shatters when given a sharp tap.

buckyball A ball-like polyhedral molecule consisting of carbon atoms of the type found in fullerenes.

C

calibration Adjusting an instrument with a standard scale of readings.

calibration curve In AAS, a graph showing the relationship between the concentration of a particular compound in a sample and the absorbance of that sample. Used to determine an unknown concentration when the absorbance of the sample has been measured.

calibration factor The amount of energy that is required to change the temperature of the water within a calorimeter by 1°C.

calorimeter An instrument designed to measure energy changes in a reaction. It is made up of an insulated container of water in which the reaction occurs, with a stirrer and thermometer to measure the temperature change during the reaction.

calorimetry The experimental method by which the heat energy released by a chemical reaction is measured.

catalysis The increase in the rate of a chemical reaction due to the presence of a catalyst.

catalyst A substance that increases the rate of a reaction but is not consumed in the reaction. The catalyst provides a new reaction pathway with a lower activation energy. May be of organic or inorganic origin.

catalytic cracking The conversion of higher molecular weight hydrocarbons from petroleum refining into smaller molecules using heat and a catalyst.

cathode ray tube A tube containing a vacuum or gas through which electron beams travel and produce visible light on a phosphorescent surface.

cation A positively charged ion, e.g. a sodium ion Na^+.

Celsius scale The temperature scale on which the freezing point of water is given a value of 0 and the boiling point a value of 100.

ceramic Relating to products made from clay and similar materials, such as pottery, brick, etc.

ceramic insulator A material with high resistance to electrical current, used to keep high-voltage power lines insulated from electricity poles and electric fence wires.

change of state When matter changes from one physical state to another.

charge imbalance When there are unequal numbers of protons and electrons in an atom.

chemical (HAZCHEM) code A system of codes and images that provides warning of hazards about items to users.

chemical change A chemical reaction. A change in the chemical composition of matter where one or more types of matter are transformed into a new type or new types of matter.

chemical energy The sum of the chemical potential energy and kinetic energy in a substance. Chemical energy is stored in bonds between atoms and molecules. The energy results from things such as attractions between electrons and protons in atoms, repulsions between nuclei, repulsions between electrons, movement of electrons, and vibrations and rotations around bonds.

chemical equation A symbolic representation of a chemical reaction using the chemical formulas of the substances involved in the reaction. A balanced chemical equation shows the relative amounts of reactants and products in the reaction. The reactants (written on the left-hand side) are connected by an arrow to the products (written on the right-hand side).

chemical formula A shorthand representation of a substance (element or compound) using chemical symbols. The chemical formula of a compound also uses numerical subscripts to convey the relative proportions of the different types of atoms in the compound.

chemical property A characteristic of a substance observed during a chemical reaction.

chemical reaction A rearrangement of atoms where one or more types of matter are transformed into a different type of matter. Typically involves the breaking and forming of chemical bonds.

chemical symbol A symbolic representation of an element, usually one or two letters, where the first letter is capitalised and the second letter is lower case, e.g. the chemical symbol for carbon is C and the chemical symbol for sodium is Na.

chromatogram The output of a chromatography procedure. In TLC and paper chromatography it is the pattern of bands or spots on the paper/plate.

chromatography A technique for separating the components of a mixture, involving the movement of the sample through the adsorbent stationary phase by a mobile phase.

claim An assertion made to influence decision-making or public debate. It represents a proposed explanation, interpretation or conclusion, and is subject to evaluation and scrutiny in scientific investigation.

coefficient Whole numbers placed in front of formulas to make the equation balance.

coefficient of determination A calculated value that indicates the ability to predict the dependent variable value from the independent variable value.

collision theory A theoretical model that accounts for the rates of chemical reactions in terms of collisions between particles occurring during a chemical reaction.

column chromatography Chromatography where the stationary phase is in a column, e.g. gas chromatography (GC) or high performance liquid chromatography (HPLC).

column graph A graph that shows the measured value of the dependent variable by the height of a column.

combustion A rapid reaction with oxygen accompanied by the release of large amounts of energy. Also called burning.

compound A pure substance composed of more than one type of atom chemically combined in fixed proportions.

concentrated solution A solution that has a relatively high ratio of solute to solvent.

concentration A measure of how much solute is dissolved in a specified volume of solution.

concentration–time curve A plot of reactant and/or product concentration versus time. It shows how the concentration of substances in a chemical reaction changes with time and can be used to determine the rate of reaction at any time.

condensation The change of physical state where a gas becomes a liquid.

condensed electron configuration A shortened way of writing electron configuration that uses the noble gas symbol before the element.

conductivity Capacity to transfer electrical current (electrical conductivity) or heat (thermal conductivity).

conductor An object or type of material that permits the flow of electric charges, e.g. a wire is an electrical conductor that can carry electricity along its length.

continuous quantitative data Data that cannot be counted; for example, the numbers between 1 and 2.

continuous variable Numerical variables that are based on a continuum in which infinite fractional values exist.

continuum (emission spectrum) The spacing between successive spectral lines within the emission spectrum becomes so small such that they are indistinguishable from one another.

controlled variable A variable that is controlled during an experiment so that it does not change and does not influence the measured results or dependent variable.

covalent bond The force of attraction formed when one or more pairs of electrons are shared between two nuclei.

covalent compound A compound formed by covalent bonds between non-metallic elements.

covalent layer lattice An arrangement of atoms in a lattice in which there are strong covalent bonds between the atoms that have formed in a layer and weak intermolecular forces between the layers.

covalent network lattice An arrangement of atoms in a lattice in which there are strong covalent bonds between the atoms in all three dimensions.

covalent network solid A giant covalent substance in which all the atoms are held together by covalent bonds to form a continuous three-dimensional structure.

crystal lattice The symmetrical three-dimensional arrangement of atoms or ions inside a crystal.

current A movement or flow of electric charges.

D

data In science, measurements of an attribute or attributes; data may be quantitative or qualitative and be from primary or secondary sources. (ACARA 2015c)

data loggers Portable tablets that record and log data acquired or measured using probes, sensors and instruments.

decomposition A reaction in which a compound is broken down into smaller parts.

delocalise Spread out.

delocalised electron An electron that is not restricted to the region between two atoms. It is not localised to a particular atom and is free to move.

density A measure of the amount of mass per unit volume. It has the SI units of kg m^{-3}, but is commonly quoted in g cm^{-3}.

dependent variable The variable that is measured or observed during an experiment, which is assumed to change due to the independent variable.

deposition The change of physical state where a gas becomes a solid.

desorption The disruption of attraction between a substance and the surface to which the substance is adsorbed.

deviation The amount that a measurement differs from a fixed value.

diamond A form of pure carbon that is the hardest naturally occurring substance.

diatomic molecule A molecule formed from two atoms only, e.g. Cl_2.

dilute solution A solution that has a relatively low ratio of solute to solvent.

dilution The addition of a solvent to a solution to reduce its concentration.

dipole The separation of positive and negative charges in a bond or molecule.

dipole–dipole forces The attractive forces between polar molecules that result from the attraction between the positive and negative ends of the dipoles.

discrete (discontinuous) data Data that can be counted, with values that are separate and distinct.

dispersion forces The attractive forces caused by temporary dipoles that are the result of random movement of the electrons surrounding the molecules.

dissociate Break up.

dissociation A process in which molecules or ionic compounds separate or split into smaller particles such as atoms or ions. Examples of dissociation reactions include the solution of NaCl solid in water, forming $Na^+(aq)$ and $Cl^-(aq)$ ions, and the reaction of HCl gas with water, forming $H^+(aq)$ and $Cl^-(aq)$.

dissolution The process of dissolving a solute in a solvent to form a solution.

dissolve To incorporate a solid or gas into a liquid so as to form a solution.

distillation A purification technique used for separating mixtures containing a liquid component by first evaporating the liquid to its gaseous state and then recondensing it back to its liquid state. Distillation uses the differences in boiling points of the components of the mixture.

double covalent bond A covalent bond in which four electrons (two electron pairs) are shared between two nuclei. It is depicted in a valence structure as two lines between the two atoms involved.

ductile Able to be drawn (stretched) into a wire.

E

effective nuclear charge The charge experienced by the valence-shell electrons in an atom. It indicates the attractive force felt by the valence electrons towards the nucleus.

elastic collision A collision in which there is no loss of kinetic energy.

electric dipole The separation of positive and negative charges in a bond or molecule.

electrode A solid conductor that makes contact with an electrolyte in an electrical circuit.

electrolyte A chemical substance that conducts electric current as a result of dissociation into positively and negatively charged ions, which migrate towards the negative and positive electrodes of an electric circuit.

electromagnetic radiation Radiant energy consisting of synchronised oscillations of electric and magnetic fields, or electromagnetic waves, propagated at the speed of light in a vacuum.

electromagnetic spectrum All possible frequencies of electromagnetic radiation shown in order of their wavelengths or frequencies.

electron A negatively charged, very light particle found in energy levels outside the nucleus; a subatomic particle.

electron configuration In the subshell (quantum mechanical) model of an atom, the electron configuration is a means of representing the number of electrons in each subshell.

electron configuration notation A written series of numbers and/or letters stating the number of electrons in each subshell.

electron density The concentration of electrons around an atom or a molecule.

electron distribution The arrangement of electrons around an atom or a molecule.

electron dot diagram See *Lewis structure*.

electron pair arrangement The distribution of pairs of electrons around an atom in a way that minimises repulsion.

electron shell A region or energy level of the atom in which electrons can be found.

electron transfer diagram A diagram that shows how electrons move from a metal atom to a non-metal to form ions.

electronegativity The ability of an atom to attract electrons towards itself within a chemical bond.

electrostatic attraction The force of attraction between a positively charged particle and a negatively charged particle.

electrostatic force The force of attraction or repulsion between particles that are the result of the charge on each particle.

element (1) A component or constituent part of a complex whole; a fundamental, essential or irreducible part of a composite entity; a pure substance containing only one type of atom (same atomic number). (2) Elements cannot be broken down into simpler substances by physical or chemical means (QCAA).

eluent The solvent that carries the components and passes through the chromatography column. It may be a liquid or a gas.

emission spectrum A spectrum produced when an element is excited by heat or radiation, then emits radiation as electrons move from the higher energy level to a lower energy level. It appears as distinct lines characteristic of the element.

empirical formula A formula that shows the simplest whole number ratio of the elements in a compound, e.g. CH_2 is the empirical formula of propene (C_3H_6).

endothermic A reaction that absorbs energy from the surroundings; ΔH is positive.

energy The capacity for doing work or generating heat.

energy level A region or electron shell of the atom in which electrons can be found.

energy profile diagram A diagram that shows the energy changes during the course of a reaction.

enthalpy Heat content. The sum of the chemical, potential and kinetic energies in a substance. Given the symbol H.

enthalpy change The difference in the total enthalpy of the products and the total enthalpy of the reactants. Given the symbol ΔH.

enthalpy level diagram A diagram that shows the energy changes during the course of a reaction.

enzyme A protein molecule that functions as a catalyst of a specific biochemical reaction. A catalyst that increases the rate of reaction.

equilibrium A state of balance in which the rate of a forward reaction or process is equal to the rate of its reverse reaction or process.

error The difference between a measurement and the true value; this is not an indication of human error or a mistake.

error bar A line drawn through a point on a graph that is parallel to one of the axes and which represents the uncertainty or variability of the data of that point.

ethics Moral principles that govern a person's behaviour or the conducting of an activity.

evaporation The change of physical state where a liquid becomes a gas.

excess reactant A reactant that is not completely consumed in a chemical reaction.

excited electron An electron that has absorbed a particular quantity of energy and moved from its ground state to a higher energy level. An atom is said to be excited when an electron is not in the lowest electron energy level possible (i.e. not in the ground state).

excited state A state where energy has been absorbed by an atom and electron(s) have moved to a higher energy level; energy will be released as it returns to its ground state.

exothermic An exothermic reaction releases energy to the surroundings; ΔH is negative.

extend To extend an experiment means to adjust the methodology to address limitations in the scope or applicability of the original data.

extrapolate Infer or estimate by extending or projecting known information; conjecture; infer from what is known; extend the application of something (e.g. a method or conclusion) to an unknown situation by assuming that existing trends will continue or similar methods will be applicable (QCAA).

F

first ionisation energy The energy required to remove one electron from an atom of an element in the gaseous state.

fluoresce To shine or glow brightly.

formula unit Chemical formula that shows the overall ratio of positive and negative ions in an ionic compound.

fossil fuel Fuel produced over a long period of time by the breakdown of organic material. This includes coal, crude oil and natural gas.

fractional distillation Separation of components of a mixture based on their boiling point.

freezing The change of physical state where a liquid becomes a solid.

freezing point The temperature at which a substance is transformed from its liquid state to its solid state and where both states coexist in equilibrium.

freezing point depression The decrease in temperature between the freezing point of a solution and the freezing point of the pure solvent.

fuel A substance that can release stored energy easily.

full equation A representation of a reaction that uses formulas.

fullerene A molecule composed entirely of carbon, in the form of a hollow sphere, tube, or other shape. Each carbon atom is bonded to three other carbon atoms.

G

gamma radiation Short wavelength, high energy electromagnetic radiation.

gas Matter that does not have a defined shape, and will expand to fill the container it is placed in. The particles in a gas move independently of one another.

gas constant The constant, R, in the ideal gas equation. $R = 8.31\ J\ K^{-1}\ mol^{-1}$ when pressure is measured in kPa, volume in L and temperature in K.

gaseous Having the characteristics of a gas; no fixed shape and takes on the shape of the space available.

giant covalent network An arrangement of atoms in which there are strong covalent bonds between the atoms forming a continuous three-dimensional network.

graph A diagram showing the relationship between variable quantities, usually two variables.

graphene A form of carbon consisting of planar sheets one atom thick in which each carbon atom is bonded to three neighbouring carbon atoms.

graphite A form of carbon in which the carbon atoms are arranged in layers.

ground state A term used to describe an atom in which the electrons occupy the lowest possible energy levels.

group (periodic table) A vertical column of elements in the periodic table.

H

Haber process The process of producing ammonia from hydrogen gas and nitrogen gas.

half-life The time taken for the number of particles emitted from a radioactive source to be reduced by half.

halogen A group 7 element—F, Cl, Br, I, At, Ts.

heat The energy transferred from one system to another because of a difference in temperature.

heat content The enthalpy of a substance. Given the symbol *H*.

heat of combustion The energy released when specified quantities (e.g. 1 mole or 1 gram) of a substance burns completely in oxygen.

heat of neutralisation The energy released, ΔH, when an acid is neutralised by a base.

heat of reaction The exchange of heat between a system and its surroundings during a chemical reaction under constant pressure. Given the symbol ΔH, and also known as the enthalpy change.

Hess's law The amount of heat energy released or absorbed in a chemical reaction is constant, irrespective of the number of steps or the kind of steps by which the reaction is carried out, provided that the same reactants and products are involved.

heterogeneous Diverse, different.
A heterogeneous substance or solution possesses two or more different types of phases in the one sample, e.g. a suspension.

heterogeneous catalyst A catalyst that has a different physical state from the reactants and products.

heterogeneous mixture A mixture consisting of two or more substances that have visibly distinguishable regions, called phases, which have different physical and chemical properties.

Higgs boson Particle that is the carrier of the Higgs field and endows subatomic particles with mass through its interactions with them.

homogeneous Uniform. The components of a homogeneous substance are uniformly distributed throughout the substance, e.g. a solution is homogeneous because the solute and the solvent cannot be distinguished from each other.

homogeneous catalyst A catalyst that has the same physical state as the reactants and products.

homogeneous mixture A mixture consisting of two or more substances but only one visibly distinct phase that has uniform physical and chemical properties throughout.

Hund's rule Describes how to arrange electrons when a *p* or *d* subshell is not full. It states that every orbital in a subshell is singly occupied before any orbital is doubly occupied.

hydrated An ion surrounded by water molecules. Hydrated ions can be found in aqueous solutions or crystalline solids.

hydride A compound in which hydrogen is bonded to another element. HF, HCl and HI are hydrides of group 17 elements.

hydrocarbon A compound that contains carbon and hydrogen only.

hydrogen bond A type of intermolecular, dipole–dipole force where a hydrogen atom is covalently bonded to a highly electronegative atom such as oxygen, nitrogen or fluorine. Due to the disparity of electronegativity values between the atoms involved, the hydrogen develops a partial positive charge and bonds to lone pairs of electrons on neighbouring atoms of oxygen, nitrogen or fluorine.

hydrogen bonding A particularly strong form of dipole–dipole force that only occurs between highly polar molecules in which a hydrogen atom is covalently bonded to an oxygen, a nitrogen or a fluorine atom.

hydronium ion The $H_3O^+(aq)$ ion.

hydroxide ion The $OH^-(aq)$ ion.

hyperbaric oxygen therapy (HBOT) A medical treatment in which patients breathe pure oxygen while inside a decompression chamber at a pressure higher than 1 atm.

hypothesise Formulate a supposition to account for known facts or observed occurrences; conjecture, theorise, speculate; especially on uncertain or tentative grounds (QCAA).

I

ideal gas A gas that obeys the gas equations at all temperatures and pressures.

ideal gas equation The equation that describes the behaviour of an ideal gas: $PV = nRT$.

immiscible Two liquids are immiscible if they cannot be mixed without separating from each other.

independent variable The variable during an experiment that is deliberately altered, or selected to be tested, that is assumed to cause a change in the dependent variable.

indicator A substance that is different colours in its acid and base forms.

inductively coupled plasma (ICP) A highly sensitive ionisation technique that when used in conjunction with mass spectrometry is capable of detecting metals and non-metals concentrations as low as one part in 10^{15}.

initial rate of reaction The instantaneous rate of reaction at time, $t = 0$.

inorganic Comprised of non-hydrocarbon chemical compounds. Has no biological origin, is formulated from materials that are not part of living organisms.

insoluble Incapable of being dissolved.

instantaneous dipole See *temporary dipole*.

instantaneous rate of reaction The rate of reaction at any time instant during the course of a chemical reaction.

intermolecular force An electrostatic force of attraction between molecules, including dipole–dipole forces, hydrogen bonds and dispersion forces.

International System (SI) A worldwide system used by scientists to measure physical properties using the metric system.

interstitial alloy An alloy made by adding smaller atoms to a metal.

intramolecular bond A force that holds the atoms within a molecule together.

ion A positively or negatively charged atom or group of atoms.

ion–dipole attraction The attraction that forms between dissociated ions and polar water molecules when an ionic solid dissolves in water.

ion–dipole interaction An electrostatic interaction between a charged ion and a molecule that has a dipole.

ionic bond A type of chemical bond that involves the electrostatic attraction between oppositely charged ions.

ionic compound A compound composed of positively charged ions (cations) and negatively charged ions (anions) arranged in a three-dimensional lattice. Ionic compounds are characterised by ionic bonds, i.e. the electrostatic attraction of ions of opposite charge.

ionic equation An equation for a reaction that only includes the ions that are involved in the reaction, e.g. $Cu^{2+}(aq) + 2OH^-(aq) \rightarrow Cu(OH)_2(s)$.

ionic radius A measurement used for the size of ions; the distance from the nucleus to the outermost electrons.

ionisation (i) The removal of one or more electrons from an atom or ion; (ii) the reaction of a molecular substance with a solvent to form ions in solution.

ionisation energy The energy required to remove one electron from an atom of an element in the gaseous state.

ionise The reaction of a molecular substance with a solvent to form ions in solution. When some polar molecules dissolve in water they ionise to form a hydronium ion, e.g. $HCl(g) + H_2O(l) \rightarrow H_3O^+(aq) + Cl^-(aq)$.

isoelectronic Two elements and/or ions that have the same electronic configurations.

isotope Atoms of an element that have the same number of protons but a different number of neutrons.

isotopic abundance The percentage abundance of a particular isotope in a sample of an element.

isotopic mass See *relative isotopic mass*.

J

joule The SI unit for energy.

K

Kelvin scale The temperature scale in which the freezing point of water is given a value of 273 and the boiling point a value of 373.

kilopascal (kPa) A common unit of pressure.

kinetic energy The energy that a particle or body has due to its motion: $KE = \frac{1}{2}mv^2$

kinetic energy distribution diagram A graph of kinetic energy against number of particles that shows the range of energies in a sample of a gas or a liquid at a given temperature. Also known as a Maxwell–Boltzmann distribution curve.

kinetic theory A theory that explains the states of matter based on the concept all matter is composed of tiny particles that are in constant motion.

L

Large Hadron Collider A massive 27 km underground particle accelerator and proton collider operated by the European Organisation for Nuclear Research (CERN).

latent heat The heat energy required to change the state of a substance without changing the temperature.

latent heat of fusion The energy required to change a fixed amount of solid to liquid at its melting point.

latent heat of vaporisation The energy required to change a fixed amount of liquid to gas at its boiling point.

lattice A regular arrangement of large numbers of atoms, ions or molecules.

law A statement describing invariable relationships between phenomena in specified conditions, frequently expressed mathematically.

law of conservation of energy The total energy of a system remains constant; energy can neither be created or destroyed, rather, it transforms from one form to another.

law of conservation of mass A scientific law that states that in any physical change or in any chemical reaction, matter can neither be created nor destroyed.

Lewis structure A representation of the electron arrangement in an atom, molecule or ion that uses dots to represent electrons and a line to represent two electrons in a covalent bond.

limewater test A test for carbon dioxide gas. The presence of carbon dioxide is detected by bubbling the gas through a calcium hydroxide solution ($Ca(OH)_2(aq)$). The limewater reacts with the carbon dioxide and turns milky.

limiting reactant A reactant that is completely consumed in a chemical reaction and that determines the amount of products formed.

line graph A graph that displays continuous data using a line from one point of measurement to the next.

line of best fit A straight line drawn to show the trend of data points plotted on a scatterplot.

line spectrum See *emission spectrum* and *absorption spectrum*.

liquid Matter that does not have a defined shape, and will take the shape of the container it is placed in. The particles in a liquid are in close contact with one another, but the arrangement is not fixed or orderly.

literature review An evaluative report that critically analyses the current body of knowledge.

logarithmic scale A nonlinear scale used to describe or display a variable that has a very large range of values. The scale uses the base 10 logarithm of the variable. An increase of 1 unit on the scale is equivalent to multiplying by 10.

lone pair A valence-shell electron pair that has not formed a bond with other atoms.

lustrous Shiny or reflective when freshly cut or polished.

Lyman series A series of spectral lines in the ultraviolet part of the hydrogen spectrum that is produced by transitions of electrons between the ground state energy level and higher energy levels of the hydrogen atom.

M

M Molar mass. The mass of one mole of a substance. See *molar mass*.

main group element An element in groups 1, 2 or 13–18 in the periodic table.

malleable Able to be bent or beaten into sheets.

mass A measure of an object's resistance to acceleration. It is related to the amount of matter that an object or particle contains. The SI unit for mass is the kilogram, kg, but the unit of gram, g, is more often used in chemistry studies.

mass number The total number of nucleons in an element's nucleus, A, i.e. the number of protons plus the number of neutrons.

mass spectrometer An instrument that measures the mass-to-charge ratio of particles.

mass spectrometry An analytical technique that uses the mass-to-charge, *m*/*z*, ratio of atoms, molecules and fragments of molecules to identify substances.

mass spectrum A plot of the isotopic mass, relative to the mass of carbon-12 taken as 12 units exactly, against the relative abundance of each isotope present in a sample.

matter A physical substance; anything that has mass and occupies space. (Macquarie 1981)

Maxwell–Boltzmann distribution curve A graph of kinetic energy against number of particles that shows the range of energies in a sample of a gas or a liquid at a given temperature. Also known as a kinetic energy distribution diagram.

mean A calculated value that represents the centre of a set of numbers that have been averaged.

measured variable A variable that cannot be controlled and so must be measured during an experiment to determine whether it influences the measured results or dependent variable.

measurement uncertainty The uncertainty in a measurement due to the precision of the measurement instrument. For an analog instrument it is usually half the smallest increment. For a digital instrument it is the smallest increment on the readout.

median The value of the middle number of a set of numbers arranged from smallest to highest number.

melting The change of physical state where a solid becomes a liquid.

melting point The equilibrium temperature of the solid and liquid states of a substance.

metal ion Metal atom that loses electrons to non-metallic atoms and so becomes positively charged.

metallic bond The electrostatic attractive forces between delocalised valence electrons and positively charged metal ions.

metallic bonding model A description that explains the properties and behaviour of metals in terms of the particles in metals.

metallic character The ease with which the atoms of an element lose electrons.

metalloid An element that displays both metallic and non-metallic properties, e.g. germanium, silicon, arsenic, tellurium.

methodology A systematic, structured approach to conducting a scientific experiment or investigation, outlining the step-by-step procedures used to gather data and apply the scientific method.

miscible Liquids that can be mixed in any ratio to form a homogeneous solution.

mixture A physical combination of two or more pure substances.

mobile phase The phase that moves through the stationary phase in a chromatographic separation.

mode The value that occurs most often in a set of values.

model In science, a representation that describes, simplifies, clarifies or provides an explanation of the workings, structure or relationships within an object, system or idea. (ACARA 2015c)

modify To change the form or qualities of something.

molar concentration See *molarity*.

molar mass The mass of one mole of a substance measured in g mol^{-1}; symbol *M*.

molar volume The volume occupied by one mole of gas at a specified set of conditions. At standard temperature (273 K) and pressure (100 kPa), the molar volume of a gas is 22.4 L mol^{-1}.

molarity The amount of solute, in moles, dissolved in 1 litre of solution (mol L^{-1}).

mole The unit for amount of substance. One mole contains 6.02×10^{23} elementary entities (e.g. atoms, molecules or ions). Abbreviated as mol.

mole ratio The ratio of species involved in a chemical reaction, based on the ratio of their coefficients in the reaction equation.

molecular compound A compound comprised of molecules.

molecular element An element comprised of molecules.

molecular formula A formula of a compound that gives the actual number and type of atoms present in a molecule. It may be the same as or different from the empirical formula.

molecule A definite and discrete group of atoms covalently bonded together.

monatomic Formed from a single atom, e.g. the oxide ion (O^{2-}).

N

N The number of particles in a sample of a substance.

N_A Avogadro's constant, 6.02×10^{23} mol^{-1}. See *Avogadro's constant*.

nanomaterial A material with features in the size range 1–100 nm.

nanoparticle A particle in the size range 1–100 nm.

nanorod A nanoscale rod in which length and width are in the range 1–100 nm. The length of the rod is 3–5 times its width.

nanotechnology Technologies manipulating structures sized 1–100 nanometres (10^{-9} to 10^{-7} m).

nanotube An allotrope of carbon that consists of layers of carbon atoms formed into long cylinders.

net dipole Uneven distribution of charge over the molecule as a whole.

neutral solution A solution in which the concentration of H_3O^+ ions equals the concentration of OH^- ions; is neither acidic nor basic. At 25°C, a neutral solution has a pH of 7.

neutralisation reaction An acid reacts with a base in stoichiometric proportions to form a salt plus water.

neutralise To react an acid with a base in stoichiometric proportions to form a solution of a salt and water.

neutron A neutral subatomic particle found in the nucleus of atoms.

noble gas An unreactive gaseous element in group 18 of the periodic table. With the exception of helium, noble gases have eight electrons in their valence shells.

noble gas notation See *condensed electron configuration*.

nominal variable Categorical variables based on a nominated category which is not dependent on order.

non-bonding electron A valence-shell electron that is not shared between atoms.

non-metal ion Non-metal atom that gains electrons from metal atoms and so becomes negatively charged.

non-polar Bonds or molecules that do not have a permanent dipole. They have an even distribution of charge.

non-polar solvent A liquid or solvent that is a compound of two or more elements whose electronegativities are almost the same, e.g. oil.

nuclear symbol notation The writing of an atom or isotope in the format ${}^{A}_{Z}\mathrm{X}$, where A = mass number, Z = atomic number and X is the chemical symbol for the element.

nucleon A particle in the nucleus; a proton or neutron.

nucleus A dense structure in the centre of the atom comprising almost all the mass of the atom in a very small volume.

O

observation Noticing details of an event or phenomenon.

octet arrangement Arrangement of electrons in atoms or ions in which there are eight electrons in the valence shell.

octet rule A rule used as part of the explanation for electron configuration and in bonding. The rule states that during chemical reactions, atoms tend to lose, gain or share electrons so that there are eight electrons in their valence shell.

orbital A three-dimensional region around a nucleus that can contain no more than two electrons.

orbital diagram A depiction of pairs of electrons as arrows pointing in opposite directions in linked boxes; grouped boxes represent subshells.

ordinal variable Categorical variables in which the order of the nominated category is important.

organic Composed of materials of biological origin.

origin The position that samples are placed to be separated by thin layer or paper chromatography.

outlier A value that 'lies outside' (is much smaller or larger than) most of the other values in a set of data (QCAA).

P

paper chromatography An analytical technique for separating and identifying mixtures which uses paper as the stationary phase.

parts per million (ppm) A unit of concentration which states the number of grams of solute in 1 million grams of solution. It is equivalent to the number of mg of solute per kg of solution.

Pascal A unit of pressure equal to one Newton per square metre.

Paschen series A series of spectral lines in the infrared part of the hydrogen spectrum that is produced by transitions of electrons between the $n = 3$ energy level and higher energy levels of the hydrogen atom.

Pauli exclusion principle In essence, this principle states that no more than two electrons can occupy the same orbital in an atom, and they must have opposite spin.

percentage composition The proportion by mass of the different elements in a compound. % by mass of an element in a compound = (mass of the element present/total mass of the compound) × 100%.

percentage yield A measure of the quantity of a product obtained from a chemical process compared to the maximum amount possible if the reaction were complete, expressed as a percentage: percentage yield = actual yield / theoretical yield × 100%.

period (periodic table) A horizontal row of elements in the periodic table. The start of a new period corresponds to the outermost electron of that element beginning a new shell.

periodic table (of elements) An arrangement of the elements in order of increasing atomic number, in which elements of similar chemical and physical properties are placed in vertical columns known as groups. More specifically, the groups are arranged according to similar valence-shell electron configurations.

periodic trend The periodic pattern of properties of the elements.

periodicity See *periodic trend*.

personal protective equipment (PPE) Equipment specifically designed and used during activities to protect the user from hazards.

pH scale A measure of acidity and the concentration of hydronium ions, in solution. Acidic solutions have a pH value less than 7 at 25°C and bases have a pH value greater than 7 (at 25°C). Mathematically, pH is defined as $\mathrm{pH} = -\log_{10}[H_3O^+]$.

phase A region of matter that is physically and chemically uniform in composition and properties. With respect to heterogeneous mixtures, a phase is physically and mechanically distinct from other phases.

phenomena Events that are not artificial and can be observed through the senses or can be scientifically described or explained (QCAA).

physical change A process where the form of matter may be changed without changing its chemical identity or its chemical composition. No new substances are formed during physical changes.

physical property A characteristic of a substance that can be observed or measured, and does not involve chemical change to the substance.

physical state Refers to the different physical forms that substances can take; most commonly as solids, liquids or gases.

pie chart A circular display of either qualitative or quantitative data showing the proportion of each data set (measurement, independent variable, observation) as a part of the whole.

plagiarism Taking someone else's ideas or work and passing it off as your own.

plasma An ionised state of matter, similar to a gas.

polar Bonds or molecules with a permanent dipole. They have an uneven distribution of charge.

polar solvent A solvent whose molecules have a permanent dipole (uneven distribution of charge).

polarisable Describes an atom or molecule whose electron cloud can be distorted to form a temporary dipole. The more polarisable the atom or molecule is, the more easily its electron cloud can be distorted and the more easily it will form a temporary dipole.

polarised Describes an atom or molecule in which the electron cloud has been distorted to form a temporary dipole.

polarity The measure of how polar a molecule or bond is. It is a measure of the unequal sharing of electrons and is the result of the difference in electronegativities of the bonded atoms.

polyatomic ion An ion that is made up of more than one element, e.g. the carbonate ion (CO_3^{2-}).

polyatomic molecule A molecule that consists of more than two atoms, e.g. H_2O.

positron emission tomography (PET) A medical imaging technique detecting positrons emitted from short-lived radionucleotides in the body.

potential energy The energy that an object or a piece of matter has due to its position or composition.

precipitate The solid formed during a reaction in which two or more solutions are mixed.

precipitation reaction A reaction between substances in solution in which one of the products is insoluble.

precision Accuracy; exactness; exact observance of forms in conduct or actions.

In science, exactness; how close two or more measurements of the same object or phenomena are to each other.

prefix A symbol written at the front of a unit to indicate that the measurement is a power of ten higher or lower than the unit itself.

pressure The force exerted per unit area over a surface.

primary data Data collected directly by a person or group. (ACARA 2015c)

primary source Information created by the person or persons directly involved in a study, investigation or experiment or observing an event. (ACARA 2015c)

principle The known cause of any effect, in a system where the variables and conditions are known.

processed data Data that has been manipulated to produce meaningful information; a set of displayed data in an appropriate form such as tables or graphs; required information that has been extracted from a set.

product A substance produced in a reaction.

property A characteristic feature of a substance or material that can be used to identify or describe matter or to distinguish one type of substance from another. Includes both physical and chemical properties.

proton A positively charged subatomic particle found in the nucleus.

pure substance Matter that has a definite and distinct set of physical and chemical properties that does not change in chemical composition from sample to sample. Pure substances cannot be broken down into simpler components by physical means and are classified as either elements or compounds.

pyramidal A molecular shape in which a central atom sits at the apex of a pyramid and is bonded to three atoms on the triangular base.

Q

qualitative analysis An analysis to determine the identity of chemical(s) present in a mixture.

qualitative data Information that is not numerical in nature (QCAA).

quanta Packets of energy released or absorbed by atoms as electrons move between energy levels.

quantitative analysis An analysis to determine the concentration of chemical(s) present in a mixture.

quantitative data Numerical information. (Taylor 1982)

quantum mechanical model A mathematical description of the behaviour of electrons in atoms that links the position of an electron to its energy level.

quantum mechanics The science of the behaviour and properties of the subatomic particles of atoms.

R

radioactive A nucleus with excess energy that can be relieved by emitting the excess energy.

radioactivity A spontaneous emission of energy or particles from a nucleus, resulting in the degradation of the nucleus.

radioisotope An isotope of a chemical element that emits radioactivity due to its unstable combination of neutrons and protons in the nucleus.

random error Uncontrollable effects of the measurement equipment, procedure and environment on a measurement result; the magnitude of random error for a measurement result can be estimated by finding the spread of values around the average of independent, repeated measurements of the quantity. (ACARA 2015c)

range The variation in values between upper and lower limits on a particular scale or the largest and smallest measurements.

rate of reaction The change in concentration of a reactant or product over a period of time (usually one second): rate of reaction = change in concentration/time.

rationale A set of reasons, or logical basis for a course of action or decision (QCAA).

raw data Unprocessed and/or unanalysed data; data that has been collected without any additional processing. (Taylor 1982)

reactant A substance present at the start of a reaction.

reaction pathway A series of chemical reactions that converts a starting material into a product in a number of steps.

reactivity The ease with which a chemical can undergo reactions.

real gas Gases that do not obey the gas laws.

redirect To adjust the methodology to explore new aspects or gain deeper insight into the phenomena observed in the initial experiment.

reference list A list of resources that were cited, or in-text referenced in the document.

refine To refine an experiment means to adjust the methodology for greater accuracy or precision, often leading to more investigable research questions.

regression The calculated estimate of the strength of a relationship between variables.

relative atomic mass The weighted average of the relative isotopic masses of the naturally occurring isotopes of an element on the scale where ^{12}C is 12 units exactly; symbol A_r.

relative formula mass The average mass of a formula unit of a substance such as an ionic compound or a covalent network substance. It is numerically equivalent to the sum of the relative atomic masses of the atoms making up the formula. Substances that contain atoms or ions bonded in lattice structures have a relative formula mass.

relative isotopic abundance A measure of how much (as a percentage) a particular isotope appears in the naturally occurring element.

relative isotopic mass The mass of an atom of the isotope relative to the mass of an atom of carbon-12 taken as 12 units exactly.

relative molecular mass The mass of a molecule in a molecular compound; symbol M_r. It is numerically equivalent to the sum of the relative atomic masses of all the atoms making up the molecule.

relative uncertainty The measured uncertainty displayed as a percentage of the measurement.

reliability In science, the likelihood that another experimenter will obtain the same results (or very similar results) if they perform exactly the same experiment under the same conditions. (ACARA 2015c, Taylor 1982)

renewable energy Energy from a source that can be replenished at the same rate as being used.

repeat trial Repeatedly conducting a process, activity or trial in an attempt to replicate the results.

replication Repeatedly conducting or choosing a process, activity or sample attempting to replicate the results, event or set-up.

research question A focused, specific and relevant query developed from a claim that directs the scientific investigation. It should address a key concept related to the claim and guide all stages of research, including inquiry, analysis, interpretation and evaluation.

retardation factor (R_f) The ratio of the distance moved by a component to the distance the solvent has moved from the origin.

risk assessment Evaluations performed to identify, assess and control hazards in a systematic way that is consistent, relevant and applicable to all school activities; requirements for risk assessments related to particular activities will be determined by jurisdictions, schools or teachers as appropriate.(ACARA 2015c)

S

safety data sheet (SDS) A document that outlines specific details about items that are required to be considered when handling the item for experimentation.

salt A substance formed from a metal or ammonium cation and an anion. Salts are the products of reactions between acids and bases, metal oxides, carbonates and reactive metals.

sample size The number of individual measurements or observations undertaken for each tested variable.

saturated solution A solution that cannot dissolve any more solute at the given temperature.

scatterplot A graph that displays the measured values for two variables plotted along two axes.

scientific journal A book containing the entire collection of work related to an experiment or investigation.

scientific method An orderly process of determining the relatedness between phenomena that were originally witnessed causing a query to develop.

scientific model A physical or conceptual representation of real phenomena or systems.

scientific notation A measured value written as a mathematical expression, as a number between 1 and 10 including decimals displaying all significant figures, multiplied by ten raised to a specific power.

scientific report A document that follows the report genre, systemically organising the main information and findings of scientific research or work.

secondary data Data collected by a person or group other than the person or group using the data. (ACARA 2015c, Macquarie 1981)

secondary source A source of information or data which was not created or measured by its author, rather cited from another.

seed crystal A small crystal from which a large crystal of the same material can typically be grown.

self-ionisation An ionisation reaction of pure water in which water behaves as both an acid and a base.

shell model The description of each electron in an atom as occupying a discrete energy level in the region around the nucleus; the movement of electrons to a different energy level involves absorbing or emitting energy. The shell model is also called the Bohr model.

shielding effect The repulsion between the inner-shell electrons and the valence shell electrons that reduces the effective nuclear charge experienced by the valence electrons.

significant figures The use of place value to represent a measurement result accurately and precisely. (ACARA 2015c)

single covalent bond A covalent bond in which two electrons are shared between two nuclei. It is depicted in a valence structure as a line between the two atoms involved.

solid Matter that has a definite shape and volume; the shape does not depend on the shape of the container. The particles in a solid are packed tightly together, often in an orderly arrangement.

solubility A measure of the amount of solute dissolved in a given amount of solvent at a given temperature.

solubility curve A graph of solubility versus temperature for a particular solute dissolved in a particular solvent.

solubility table A reference table that can be used to predict the solubility of ionic compounds.

soluble Capable of being dissolved or liquefied.

solute A substance that dissolves in a solvent, e.g. sugar is the solute when it dissolves in water.

solution A homogeneous mixture of a solute dissolved in a solvent.

solution calorimeter An insulated container that holds a known volume of water and in which a reaction in solution, such as dissolution of a solid or a neutralisation reaction, can be carried out.

solvent A substance, usually a liquid, which is able to dissolve a solute to form a solution. Water is a very good solvent.

solvent front The wet edge or border of the solvent as it moves through the paper or plate in chromatography.

specific heat capacity The amount of thermal energy transfer necessary to raise the temperature of one kilogram of a substance by one degree.

spectator ion An ion that remains in solution and is unchanged in the course of a reaction. Spectator ions are not included in ionic equations.

spectrometric technique A quantitative technique that analyses the way that radiation, such as light and radio waves, interacts with matter.

spectrometry A technique that produces quantitative results and involves the measurement of the interactions of radiation (for example, light) with matter.

spectroscopic technique A qualitative technique that analyses the way that radiation, such as light and radio waves, interacts with matter.

spectroscopy Study of the absorption and emission of light and other radiation, which produces qualitative results.

standard Chemical of known composition used for comparison.

standard solution A solution that has an accurately known concentration.

standard temperature and pressure (STP) Conditions of temperature and pressure relevant to a gas, where the temperature is 0°C (273 K) and pressure is 100 kPa.

state of matter Three physical forms that matter can occur in; solid, liquid, and gas.

state symbol Symbols used in chemical equations to indicate the state of a reactant or product chemical.

stationary phase In chromatography, a solid or a liquid on a solid support that selectively adsorbs components of a mixture as they are carried along by the mobile phase.

steel A generally hard, strong, durable and not malleable alloy of iron and carbon, usually containing 0.2–1.5% carbon, often with other constituents such as manganese, chromium, nickel, molybdenum, copper, tungsten, cobalt or silicon, depending on the desired alloy properties.

stoichiometry The calculation of relative amounts of reactants and products in a chemical reaction. Chemical equations give the ratios of the amounts (moles) of the reactants and products.

strong acid An acid that is also a strong electrolyte, undergoing complete ionisation when dissolved in water.

strong base A base that is also a strong electrolyte, undergoing complete dissociation when dissolved in water.

strong electrolyte A substance that, when dissolved in water, completely ionises or completely dissociates into ions.

subatomic particle A particle inside the atom, including protons, neutrons and electrons.

sublimation The process by which a substance goes directly from the solid state to the gaseous state, without passing through a liquid state.

subshell A part of a shell (energy level) containing orbitals; subshells are named *s*, *p*, *d*, *f* or *g*.

substitutional alloy An alloy made from elements of similar chemical properties and size.

substrate A reactant in a reaction that is catalysed by an enzyme.

supersaturated solution An unstable solution that has more solute dissolved at a given temperature than a saturated solution.

surface area The area of all surfaces of the substance that is exposed to the other reactants. This is proportional to the amount of particles available at the surface to react.

surface tension The resistance of a liquid to increasing its surface area.

surroundings The rest of the universe around a chemical reaction.

symmetrical molecule A molecule in which the polar bonds are evenly (or symmetrically) distributed. The bond dipoles cancel out and no net dipole is formed.

system A group of interacting objects, materials or processes that form an integrated whole; systems can be open or closed. (ACARA 2015c)

systematic error An error that is affected by the accuracy of a measurement process that causes readings to deviate from the accepted value by a consistent amount each time a measurement is made. (Taylor 1982)

T

temperature A measure of the average kinetic energy of the particles of an object.

temporary dipole A dipole that forms due to random movement of the electrons surrounding the molecule.

tensile strength The maximum resistance of a material to a force that is pulling it apart before it breaks, measured as the maximum stress the material can withstand without tearing.

tetrahedral Having the shape of a tetrahedron—the triangular pyramid with four faces that are equilateral triangles.

tetrahedral shape The shape of a molecule with a central atom surrounded by four other atoms that sit at the corners of a tetrahedron. The bond angle between any two outer atoms and the central atom is 109.5°.

theoretical yield The mass of product that would be formed if the limiting reagent reacted fully. The mass that is expected for a particular product in a chemical reaction, based on the mass of limiting reactant used.

theory In science, a set of concepts, claims and/or laws that can be used to explain and predict a wide range of related observed or observable phenomena; theories are typically founded on clearly identified assumptions, are testable, produce reproducible results and have explanatory power. (ACARA 2015c)

thermochemical equation A chemical equation that includes the enthalpy change of the reaction, ΔH.

thermochemistry The study of energy changes that occur during chemical reactions.

thin-layer chromatography An analytical technique that uses a thin layer (such as silica) spread on a glass or plastic plate to separate a mixture.

three-dimensional lattice A regular arrangement, which has depth, height and width, of large numbers of atoms, ions or molecules.

transition metal An element in groups 3–12 in the periodic table.

transition state An arrangement of atoms in a reaction that occurs when sufficient energy is absorbed for the activation energy to be reached. It represents the stage of maximum potential energy in the reaction. Bond breaking and bond forming are both occurring at this stage, and the arrangement of atoms is unstable.

trend line A line drawn onto a graph to accurately display a relationship between the variables.

trigonal planar A molecular shape in which a central atom is bonded to three atoms that form a triangle in one plane.

triple covalent bond A covalent bond in which six electrons (three electron pairs) are shared between two nuclei. It is depicted in a valence structure as three lines between the two atoms involved.

U

uncertainty Range of values within which the true value is thought to be. See also *measurement uncertainty* and *uncertainty of the mean*.

uncertainty of the mean The uncertainty associated with the average of several measurements. It is half the range of the set of measurements.

unsaturated solution A solution that contains less solute dissolved at a given temperature than a saturated solution.

V

valence electron An electron found in the valence shell, the outermost electron shell in an atom or ion.

valence shell The outermost shell of an atom that contains electrons.

valence shell electron pair repulsion (VSEPR) theory A model used to predict the shapes of molecules by assuming that the valence electron pairs surrounding an atom repel each other, and therefore adopt an arrangement that minimises this repulsion. The shape of the molecule is then determined by considering the positions of the bonded atoms.

validity In science, the extent to which tests measure what was intended; the extent to which data, inferences and actions produced from tests and other processes are accurate. (ACARA 2015c)

vaporisation Conversion of a solid or a liquid into a gas. Evaporation and boiling are both types of vaporisation.

vapour The gaseous state of a substance.

vapour pressure The pressure exerted by a vapour in equilibrium with its liquid in a closed container; vapour pressure is temperature dependent.

variable The factors that can change during an experiment or investigation.

viscosity A measure of a liquid's resistance to flow.

volume The physical space occupied by matter. The SI unit for volume is the cubic metre (m^3) but units of litres (L) and millilitres (mL) are commonly used in chemistry.

W

wavelength The distance between two successive identical points on a wave.

weak acid An acid that is also a weak electrolyte, undergoing partial ionisation when dissolved in water.

weak base A base that is also a weak electrolyte, undergoing partial ionisation when dissolved in water.

weak electrolyte A substance that, when dissolved in water, only slightly ionises or only slightly dissociates into ions.

wedge-dash notation A three-dimensional representation of a molecule in which lines are used to represent bonds in the plane of the page; wedges are used to represent bonds that extend out of the page towards the viewer and dashes are used to represent bonds that extend into the page and away from the viewer.

weighted average A weighted average takes into consideration the proportion of the entire amount that each substance provides, rather than assuming each substance contributes equally to the entire amount.

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Attributions

The following abbreviations are used in this list: t = top, b = bottom, l = left, r = right, c = centre.

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Groups

Periods

s BLOCK

p BLOCK

d BLOCK

f BLOCK

ATOMIC NUMBER → 12 24.31 ← RELATIVE ATOMIC MASS (bracketed indicates most stable isotope)
SYMBOL → Mg 1090 ← BOILING POINT °C
650 ← MELTING POINT °C
1.3 ← ELECTRONEGATIVITY
ELECTRON STRUCTURE → [Ne]3s²
Magnesium

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1								1 1.008 H -252.9 -259 2.2 1s¹ Hydrogen									2 4.003 He -268.9 -272 - 1s² Helium
2	3 6.941 Li 1342 180 1.0 1s²2s¹ Lithium	4 9.012 Be 2468 1287 1.6 1s²2s² Beryllium										5 10.81 B 4000 2077 2.0 1s²2s²2p¹ Boron	6 12.01 C 4827 3500 2.6 1s²2s²2p² Carbon	7 14.01 N -195.8 -210 3.0 1s²2s²2p³ Nitrogen	8 16.00 O -183 -219 3.4 1s²2s²2p⁴ Oxygen	9 19.00 F -188.1 -220 4.0 1s²2s²2p⁵ Fluorine	10 20.18 Ne -246 -249 - 1s²2s²2p⁶ Neon
3	11 22.99 Na 882.9 97.8 0.9 [Ne]3s¹ Sodium	12 24.31 Mg 1090 650 1.3 [Ne]3s² Magnesium										13 26.98 Al 2519 660.3 1.6 [Ne]3s²3p¹ Aluminium	14 28.09 Si 3265 1414 1.9 [Ne]3s²3p² Silicon	15 30.97 P 280.5 44.2 2.2 [Ne]3s²3p³ Phosphorus	16 32.07 S 444.6 115.2 2.6 [Ne]3s²3p⁴ Sulfur	17 35.45 Cl -34 -102 3.2 [Ne]3s²3p⁵ Chlorine	18 39.95 Ar -185.8 -189 - [Ne]3s²3p⁶ Argon
4	19 39.10 K 758.8 63.4 0.8 [Ar]4s¹ Potassium	20 40.08 Ca 1484 842 1.0 [Ar]4s² Calcium	21 44.96 Sc 2836 1541 1.4 [Ar]3d¹4s² Scandium	22 47.87 Ti 3287 1670 1.5 [Ar]3d²4s² Titanium	23 50.94 V 3407 1910 1.6 [Ar]3d³4s² Vanadium	24 52.00 Cr 2671 1907 1.7 [Ar]3d⁵4s¹ Chromium	25 54.94 Mn 2061 1246 1.6 [Ar]3d⁵4s² Manganese	26 55.85 Fe 2861 1538 1.8 [Ar]3d⁶4s² Iron	27 58.93 Co 2927 1495 1.9 [Ar]3d⁷4s² Cobalt	28 58.69 Ni 2913 1455 1.9 [Ar]3d⁸4s² Nickel	29 63.55 Cu 2560 1085 1.9 [Ar]3d¹⁰4s¹ Copper	30 65.38 Zn 907 419.5 1.6 [Ar]3d¹⁰4s² Zinc	31 69.72 Ga 2229 27.8 1.8 [Ar]3d¹⁰4s²4p¹ Gallium	32 72.64 Ge 2833 938.2 2.0 [Ar]3d¹⁰4s²4p² Germanium	33 74.92 As 613 816.8 2.2 [Ar]3d¹⁰4s²4p³ Arsenic	34 78.96 Se 684.8 220.8 2.6 [Ar]3d¹⁰4s²4p⁴ Selenium	35 79.90 Br 58.8 -7.1 3.0 [Ar]3d¹⁰4s²4p⁵ Bromine	36 83.80 Kr -153.4 -157 - [Ar]3d¹⁰4s²4p⁶ Krypton
5	37 85.47 Rb 687.8 39 0.8 [Kr]5s¹ Rubidium	38 87.61 Sr 1377 769 1.0 [Kr]5s² Strontium	39 88.91 Y 3345 1522 1.2 [Kr]4d¹5s² Yttrium	40 91.22 Zr 4406 1854 1.3 [Kr]4d²5s² Zirconium	41 92.91 Nb 4741 2477 1.6 [Kr]4d⁴5s¹ Niobium	42 95.96 Mo 4639 2622 2.2 [Kr]4d⁵5s¹ Molybdenum	43 (98) Tc 4262 2157 2.1 [Kr]4d⁵5s² Technetium	44 101.1 Ru 4147 2333 2.2 [Kr]4d⁷5s¹ Ruthenium	45 102.9 Rh 3695 1963 2.3 [Kr]4d⁸5s¹ Rhodium	46 106.4 Pd 2963 1555 2.2 [Kr]4d¹⁰5s⁰ Palladium	47 107.9 Ag 2162 961.8 1.9 [Kr]4d¹⁰5s¹ Silver	48 112.4 Cd 766.8 321.1 1.7 [Kr]4d¹⁰5s² Cadmium	49 114.8 In 2072 156.6 1.8 [Kr]4d¹⁰5s²5p¹ Indium	50 118.7 Sn 2602 231.9 2.0 [Kr]4d¹⁰5s²5p² Tin	51 121.8 Sb 1587 630.6 2.0 [Kr]4d¹⁰5s²5p³ Antimony	52 127.6 Te 987.8 449.5 2.1 [Kr]4d¹⁰5s²5p⁴ Tellurium	53 126.9 I 184.4 113.7 2.7 [Kr]4d¹⁰5s²5p⁵ Iodine	54 131.3 Xe -108.1 -112 2.6 [Kr]4d¹⁰5s²5p⁶ Xenon
6	55 132.9 Cs 670.8 28.5 0.8 [Xe]6s¹ Caesium	56 137.3 Ba 1845 727 0.9 [Xe]6s² Barium	57 138.9 La 2464 920 1.1 [Xe]5d¹6s² Lanthanum	72 178.5 Hf 4600 2233 1.3 [Xe]4f¹⁴5d²6s² Hafnium	73 180.9 Ta 5455 3017 1.5 [Xe]4f¹⁴5d³6s² Tantalum	74 183.9 W 5555 3414 1.7 [Xe]4f¹⁴5d⁴6s² Tungsten	75 186.2 Re 5596 3454 1.9 [Xe]4f¹⁴5d⁵6s² Rhenium	76 190.2 Os 5008 3033 2.2 [Xe]4f¹⁴5d⁶6s² Osmium	77 192.2 Ir 4428 2446 2.2 [Xe]4f¹⁴5d⁷6s² Iridium	78 195.1 Pt 3825 1768 2.2 [Xe]4f¹⁴5d⁹6s¹ Platinum	79 197.0 Au 2836 1064 2.4 [Xe]4f¹⁴5d¹⁰6s¹ Gold	80 200.6 Hg 356.6 -38.8 1.9 [Xe]4f¹⁴5d¹⁰6s² Mercury	81 204.4 Tl 1473 303.8 1.8 [Xe]4f¹⁴5d¹⁰6s²6p¹ Thallium	82 207.2 Pb 1749 327.5 1.8 [Xe]4f¹⁴5d¹⁰6s²6p² Lead	83 209.0 Bi 1564 271.4 1.9 [Xe]4f¹⁴5d¹⁰6s²6p³ Bismuth	84 (210) Po 962 253.8 2.0 [Xe]4f¹⁴5d¹⁰6s²6p⁴ Polonium	85 (210) At 366.8 301.8 2.2 [Xe]4f¹⁴5d¹⁰6s²6p⁵ Astatine	86 (222) Rn -61.8 -71.2 - [Xe]4f¹⁴5d¹⁰6s²6p⁶ Radon
7	87 (223) Fr 676.8 27 0.7 [Rn]7s¹ Francium	88 (226) Ra 1140 699.8 0.9 [Rn]7s² Radium	89 (227) Ac 3200 1050 1.1 [Rn]6d¹7s² Actinium	104 (261) Rf - - - [Rn]5f¹⁴6d²7s² Rutherfordium	105 (262) Db - - - [Rn]5f¹⁴6d³7s² Dubnium	106 (266) Sg - - - [Rn]5f¹⁴6d⁴7s² Seaborgium	107 (264) Bh - - - [Rn]5f¹⁴6d⁵7s² Bohrium	108 (267) Hs - - - [Rn]5f¹⁴6d⁶7s² Hassium	109 (268) Mt - - - [Rn]5f¹⁴6d⁷7s² Meitnerium	110 (271) Ds - - - [Rn]5f¹⁴6d⁸7s² Darmstadtium	111 (272) Rg - - - [Rn]5f¹⁴6d⁹7s² Roentgenium	112 (285) Cn - - - [Rn]5f¹⁴6d¹⁰7s² Copernicium	113 (284) Nh - - - [Rn]5f¹⁴6d¹⁰7s²7p¹ Nihonium	114 (289) Fl - - - [Rn]5f¹⁴6d¹⁰7s²7p² Flerovium	115 (289) Mc - - - [Rn]5f¹⁴6d¹⁰7s²7p³ Moscovium	116 (292) Lv - - - [Rn]5f¹⁴6d¹⁰7s²7p⁴ Livermorium	117 (294) Ts - - - [Rn]5f¹⁴6d¹⁰7s²7p⁵ Tennessine	118 (294) Og - - - [Rn]5f¹⁴6d¹⁰7s²7p⁶ Oganesson

	58	59	60	61	62	63	64	65	66	67	68	69	70	71
	140.1 Ce 3443 799 1.1 [Xe]4f¹5d¹6s² Cerium	140.9 Pr 3520 931 1.1 [Xe]4f³6s² Praseodymium	144.2 Nd 3074 1016 1.1 [Xe]4f⁴6s² Neodymium	(145) Pm 3000 1042 - [Xe]4f⁵6s² Promethium	150.4 Sm 1794 1072 1.1 [Xe]4f⁶6s² Samarium	152.0 Eu 1794 1072 - [Xe]4f⁷6s² Europium	157.3 Gd 3273 1313 1.2 [Xe]4f⁷5d¹6s² Gadolinium	158.9 Tb 3230 1359 - [Xe]4f⁹6s² Terbium	162.5 Dy 2567 1412 1.2 [Xe]4f¹⁰6s² Dysprosium	164.9 Ho 2700 1472 1.2 [Xe]4f¹¹6s² Holmium	167.3 Er 2868 1529 1.2 [Xe]4f¹²6s² Erbium	168.9 Tm 1950 1545 1.3 [Xe]4f¹³6s² Thulium	173.1 Yb 1196 824 - [Xe]4f¹⁴6s² Ytterbium	175.0 Lu 3402 1663 1.0 [Xe]4f¹⁴5d¹6s² Lutetium
	90 232.0 Th 4875 1750 1.3 [Rn]6d²7s² Thorium	91 231.0 Pa - 1572 1.5 [Rn]5f²6d¹7s² Protactinium	92 238.0 U 4131 1135 1.7 [Rn]5f³6d¹7s² Uranium	93 (237) Np 3902 644 1.3 [Rn]5f⁴6d¹7s² Neptunium	94 (244) Pu 3228 640 1.3 [Rn]5f⁶6d⁰7s² Plutonium	95 (243) Am 2011 1176 - [Rn]5f⁷6d⁰7s² Americium	96 (247) Cm 3110 1340 - [Rn]5f⁷6d¹7s² Curium	97 (247) Bk - 986 - [Rn]5f⁹6d⁰7s² Berkelium	98 (251) Cf - 900 - [Rn]5f¹⁰6d⁰7s² Californium	99 (252) Es - - - [Rn]5f¹¹6d⁰7s² Einsteinium	100 (257) Fm - - - [Rn]5f¹²6d⁰7s² Fermium	101 (258) Md - 827 - [Rn]5f¹³6d⁰7s² Mendelevium	102 (259) No - - - [Rn]5f¹⁴6d⁰7s² Nobelium	103 (262) Lr - - - [Rn]5f¹⁴6d¹7s² Lawrencium